Progress in *Ab Initio* Methods for Open-Shell Nuclei

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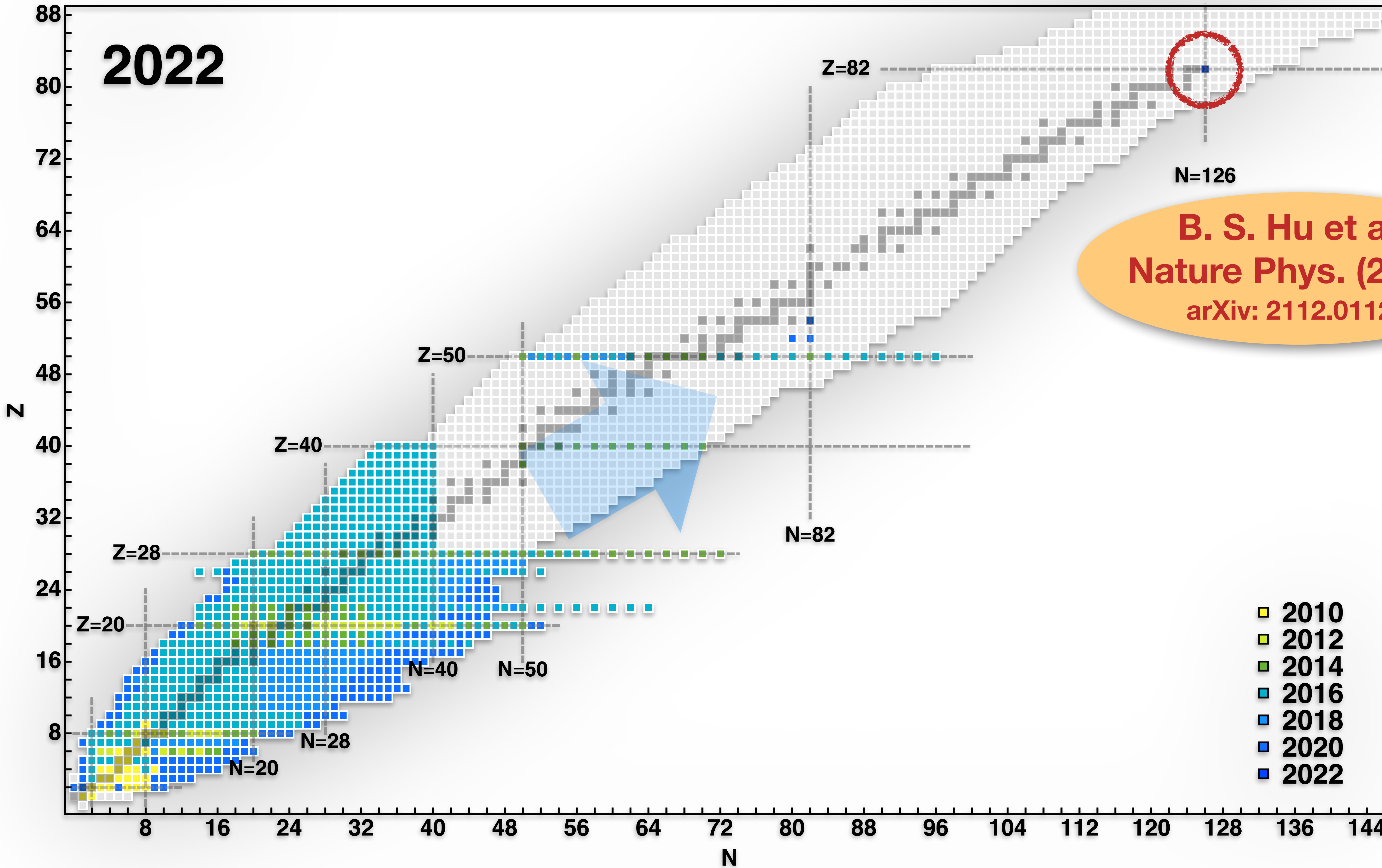
Progress in *Ab Initio* Calculations

[cf. HH, Front. Phys. ***8****, 379 (2020)]*



B. S. Hu et al., Nature Phys. (2022), arXiv: 2112.01125

(Multi-Reference) In-Medium Similarity Renormalization Group

HH, Phys. Scripta **92**, 023002 (2017)

HH, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tuskiyama, Phys. Rept. **621**, 165 (2016)

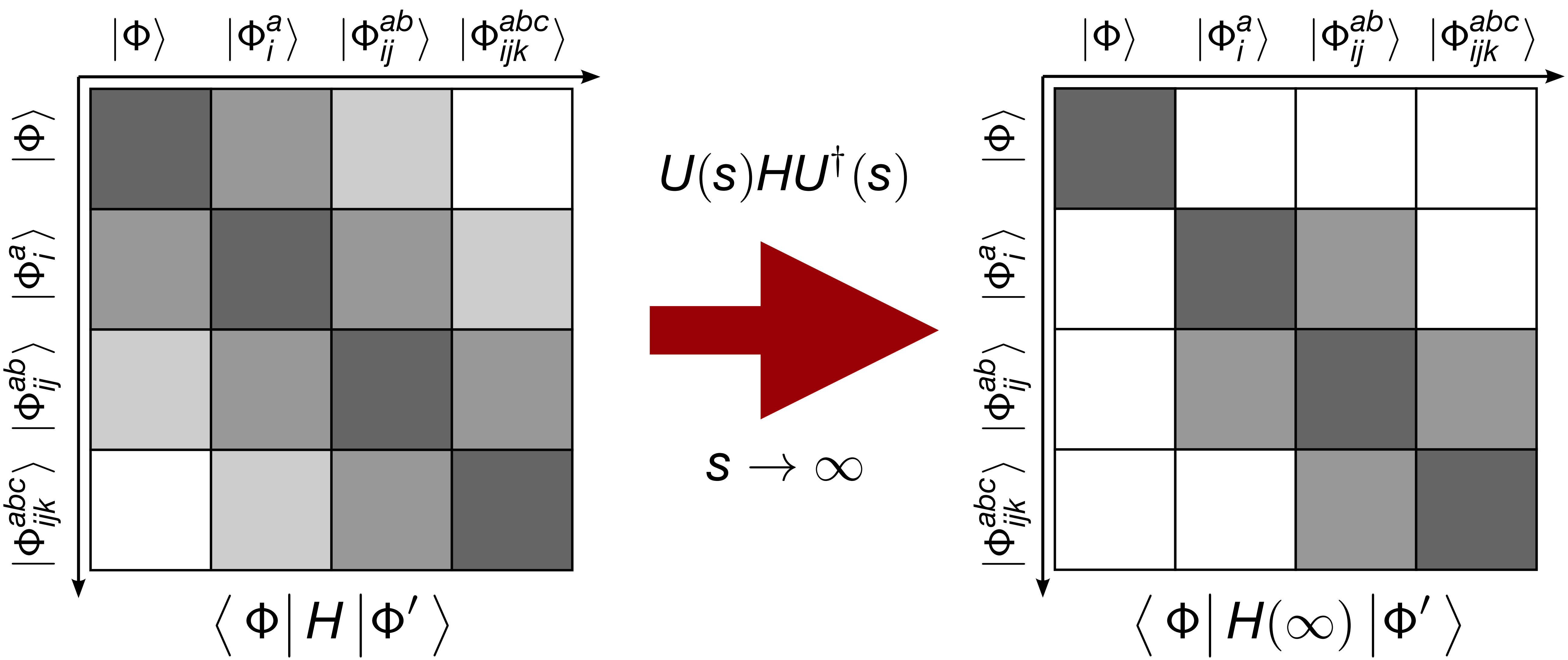
HH, S. K. Bogner, T. Morris, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. C **90**, 041302 (2014)

HH, S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. Lett **110**, 242501 (2013)

K. Tsukiyama, S. K. Bogner, A. Schwenk, PRL **106**, 222502 (2011)

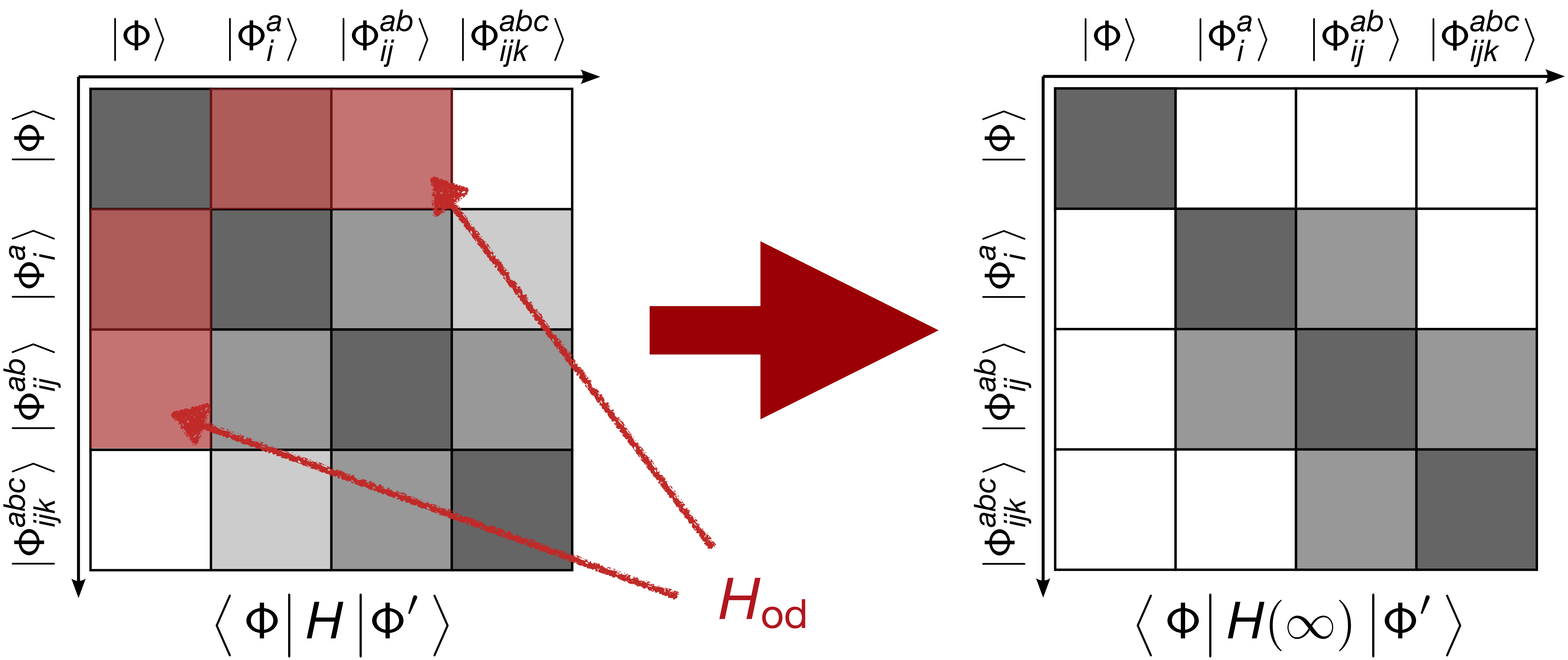
S. K. Bogner, R. J. Furnstahl, and A. Schwenk, Prog. Part. Nucl. Phys. **65**, 94

Decoupling in A-Body Space



goal: decouple reference state $|\Phi\rangle$ from excitations

Flow Equation

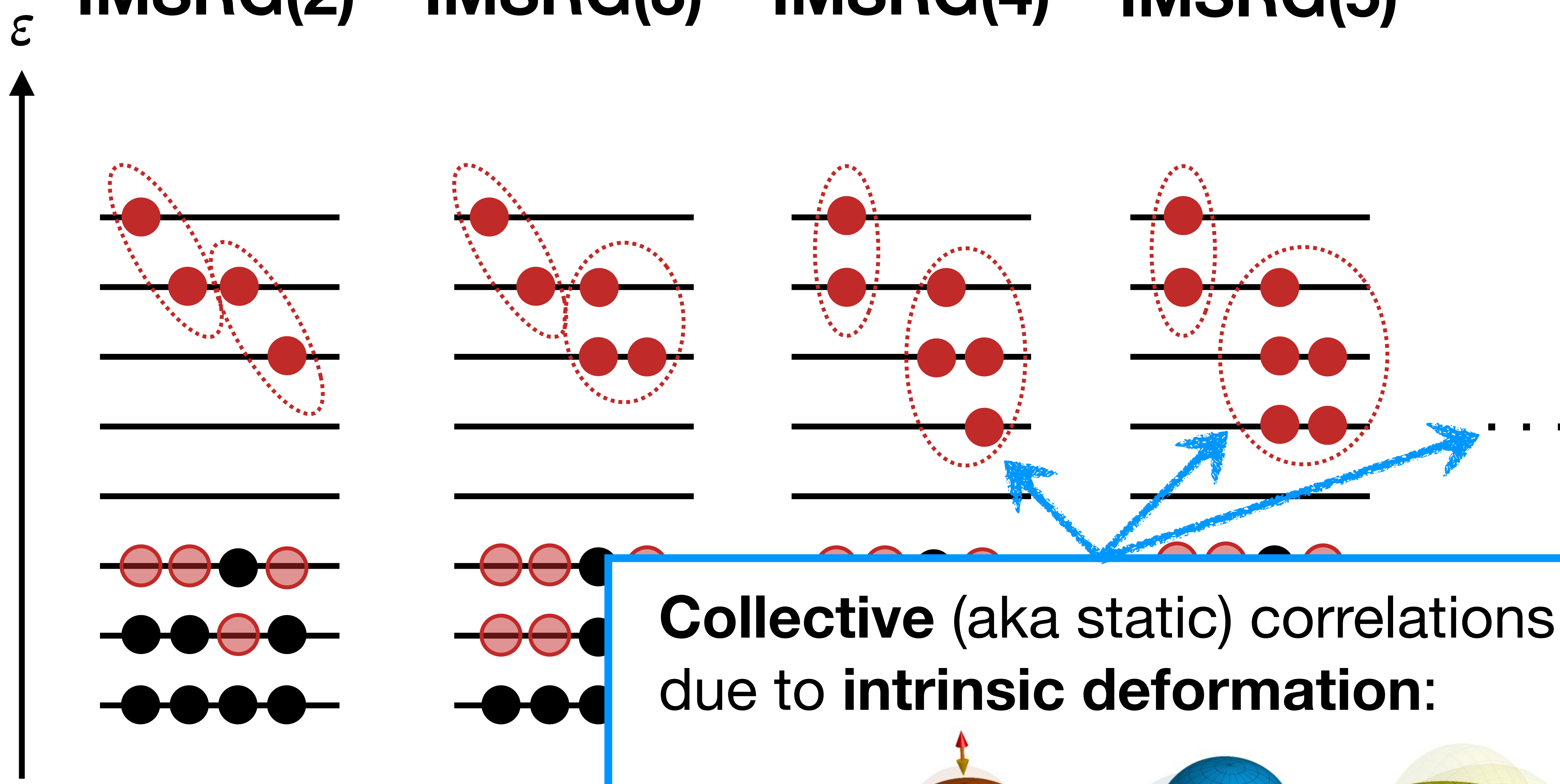


$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right],$$

Operators
truncated at **two-body level** -
matrix is never constructed explicitly!

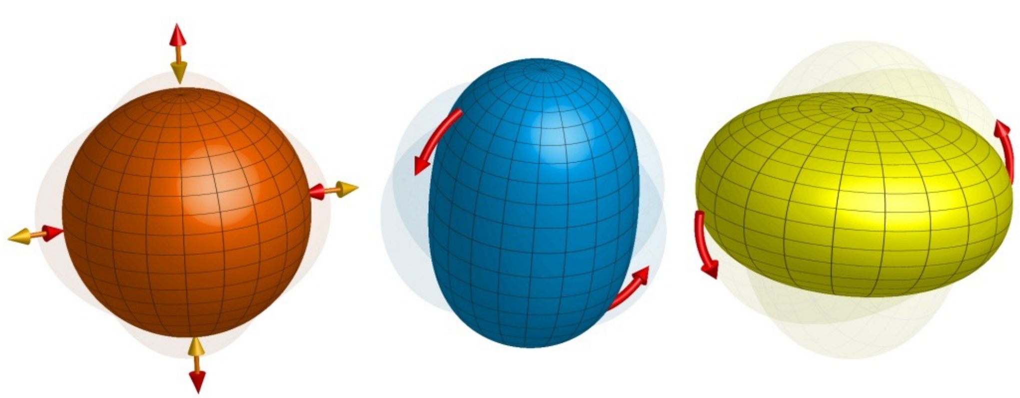
Correlated Reference States

IMSRG(2) **IMSRG(3)** **IMSRG(4)** **IMSRG(5)**

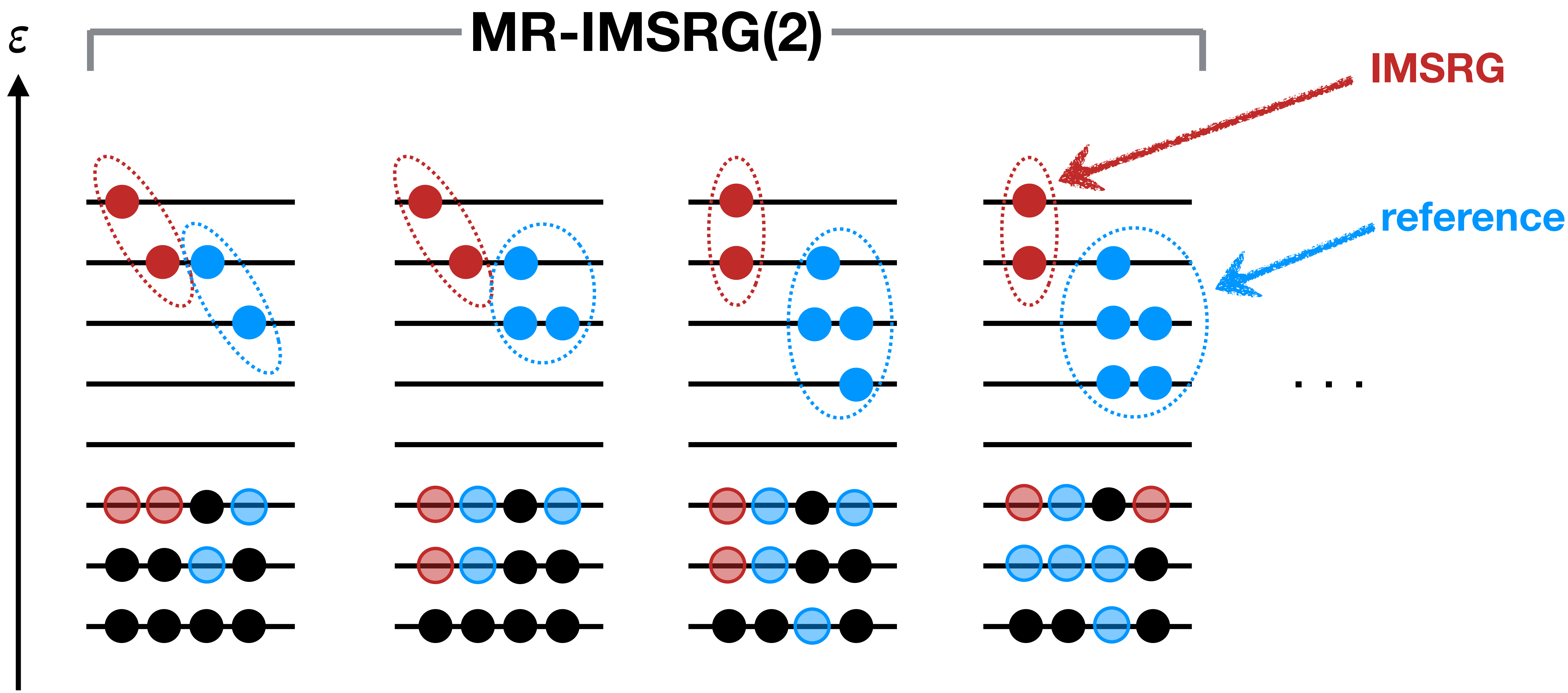


“standard” IMS
Slater determinan

Collective (aka static) correlations, e.g. due to **intrinsic deformation**:

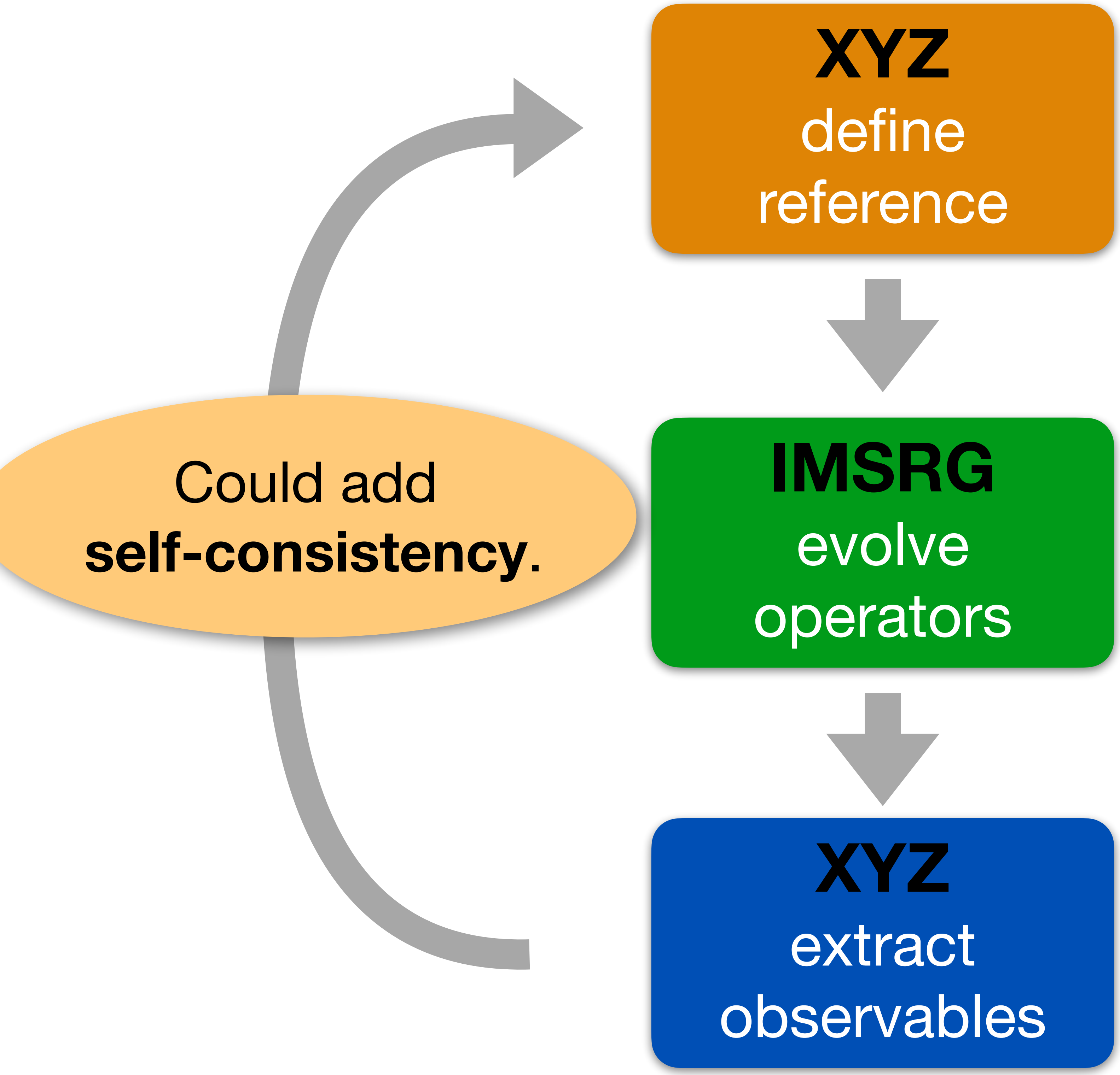


Correlated Reference States



MR-IMSRG: build correlations on top of **already correlated** state (e.g., from a method that describes static correlation well)

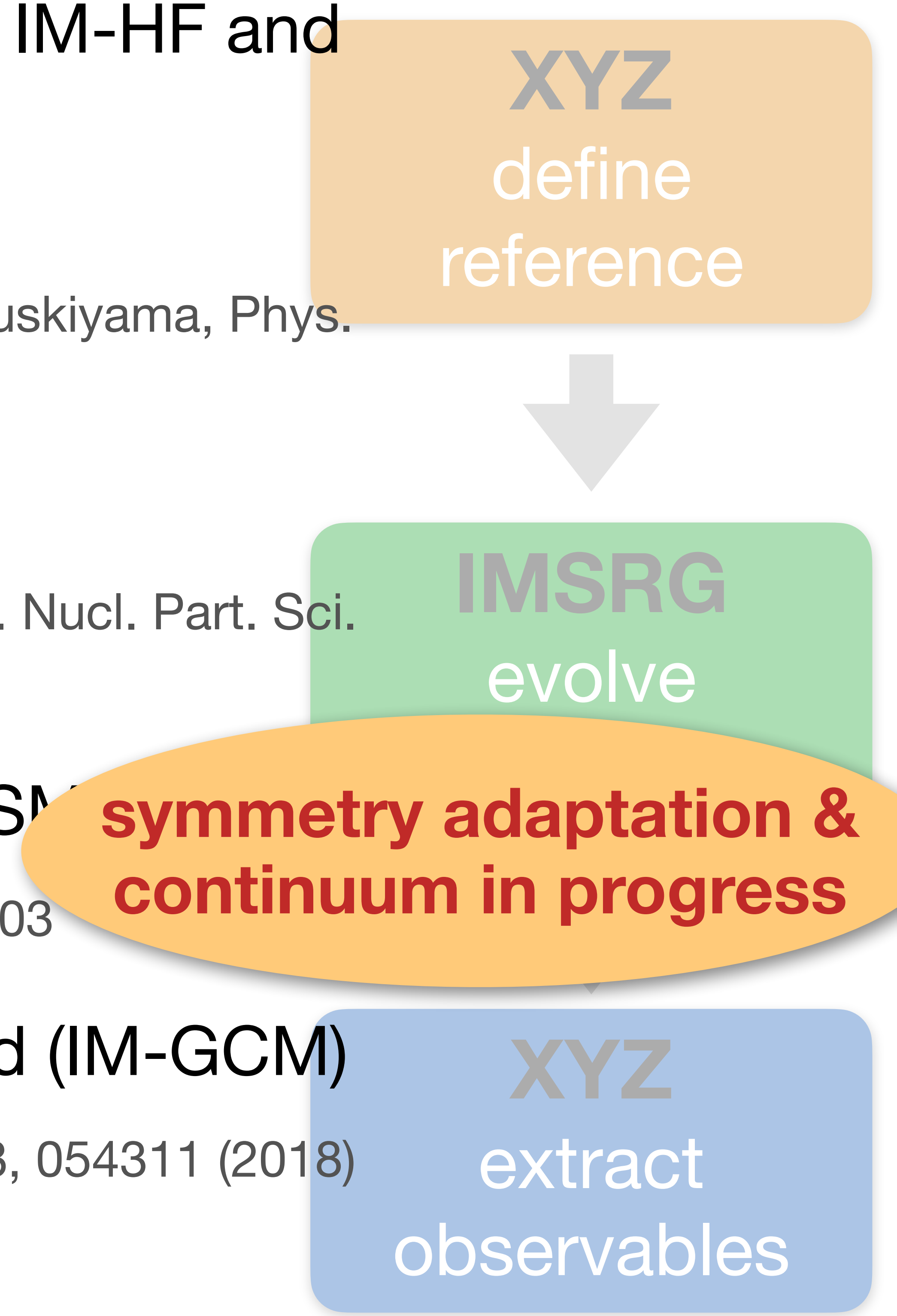
IMSRG-Improved Methods



* mean field or **explicitly correlated**

IMSRG-Improved Methods

- IMSRG for closed and open-shell nuclei: IM-HF and IM-PHFB
  - HH, Phys. Scripta, Phys. Scripta 92, 023002 (2017)
  - HH, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tuskiyama, Phys. Rept. 621, 165 (2016)
- Valence-Space IMSRG (VS-IMSRG)
  - S. R. Stroberg, HH, S. K. Bogner, J. D. Holt, Ann. Rev. Nucl. Part. Sci. **69**, 165
- In-Medium No Core Shell Model (IM-NCSM)
  - E. Gebrerufael, K. Vobig, HH, R. Roth, PRL **118**, 152503
- In-Medium Generator Coordinate Method (IM-GCM)
  - J. M. Yao, J. Engel, L. J. Wang, C. F. Jiao, HH PRC 98, 054311 (2018)
  - J. M. Yao et al., PRL 124, 232501 (2020)



Merging IMSRG and CI: Valence-Space IMSRG

Review:

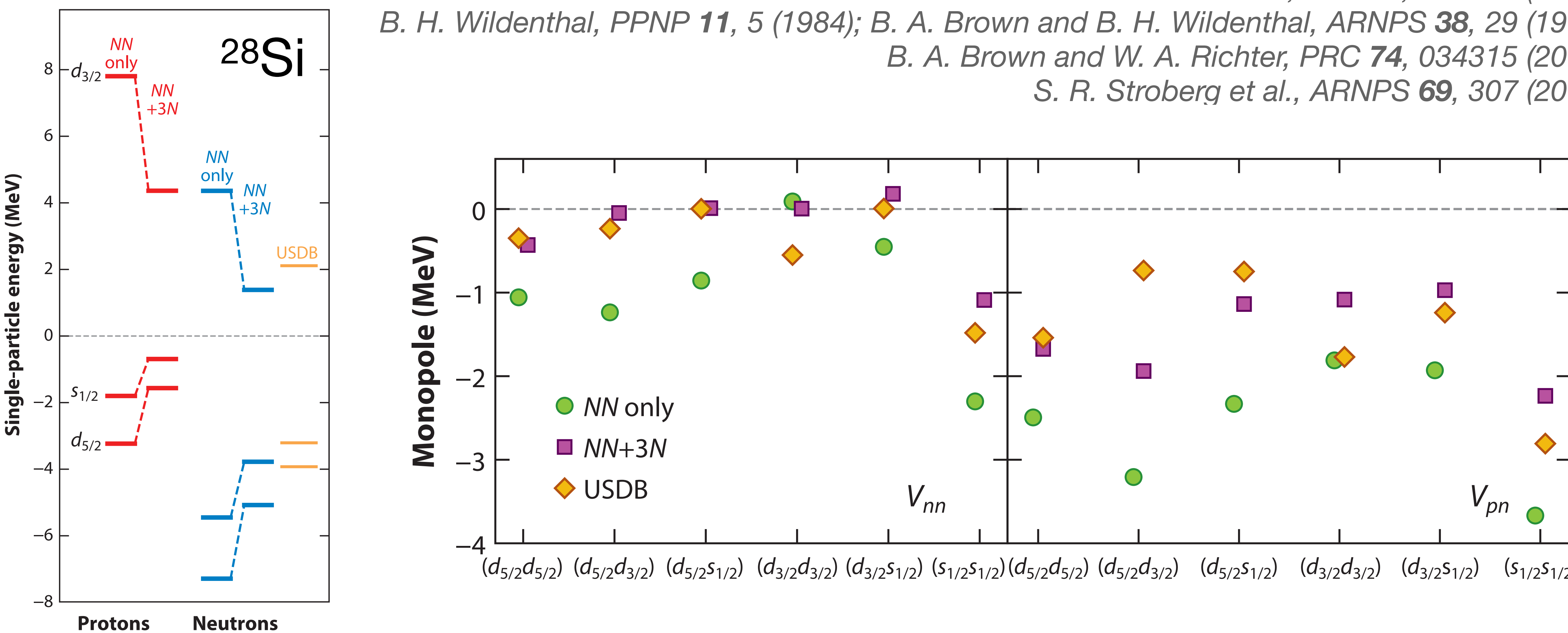
S. R. Stroberg, HH, S. K. Bogner, and J. D. Holt, Ann. Rev. Part. Nucl. Sci. **69**, 165 (2019)

Full CI:

E. Gebrerufael, K. Vobig, HH, and R. Roth, Phys. Rev. Lett. **118**, 152503 (2017)

Insights on Effect of 3N Forces

A. Zuker, PRL **92**, 042502 (2003)
B. H. Wildenthal, PPNP **11**, 5 (1984); B. A. Brown and B. H. Wildenthal, ARNPS **38**, 29 (1988)
B. A. Brown and W. A. Richter, PRC **74**, 034315 (2006)
S. R. Stroberg et al., ARNPS **69**, 307 (2019)

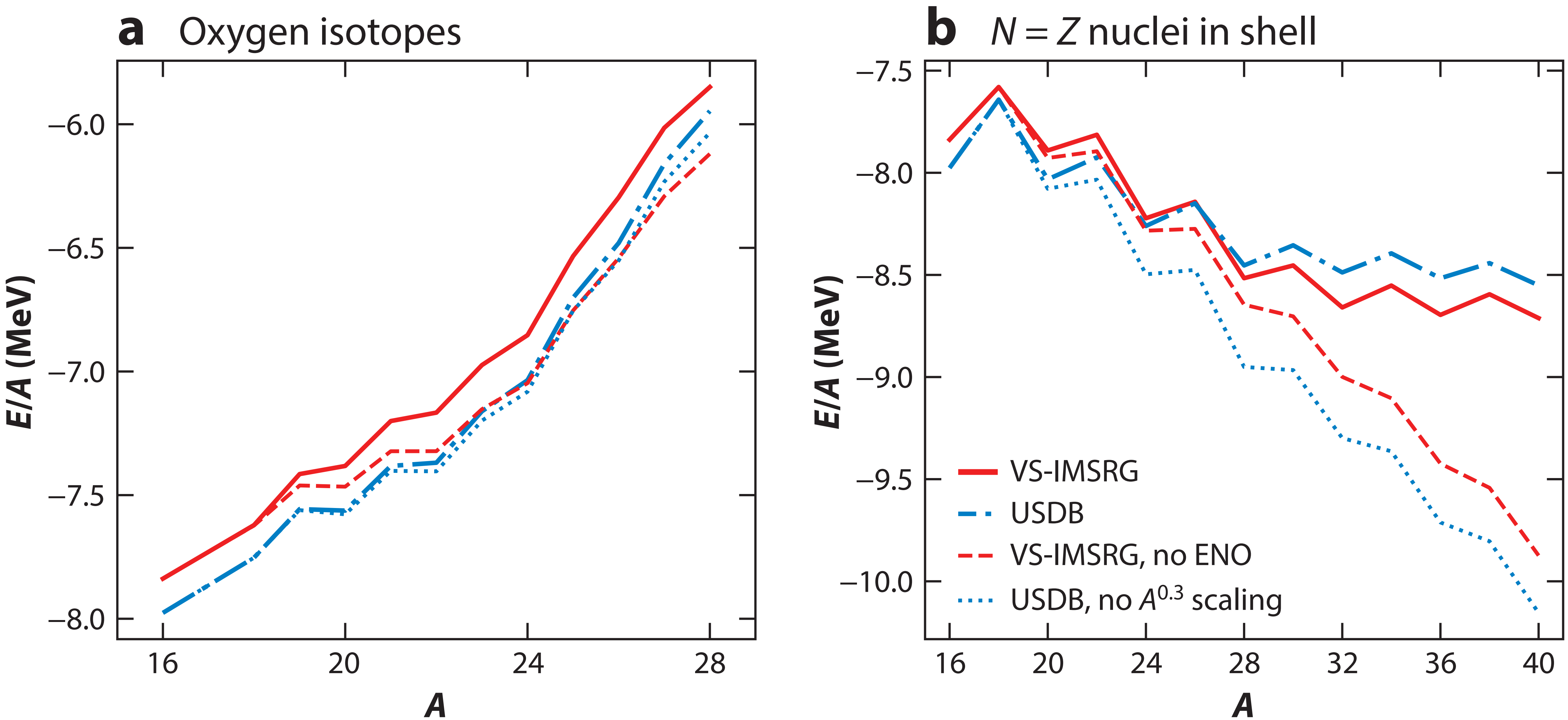


- effects of 3N forces incorporated into residual interaction via **monopole corrections** (Zuker) and $A^{0.3}$ **scaling** (Brown & Wildenthal)

- included in VS-IMSRG through **normal ordering**, but no "simple" A-dependence - partitioning of H not unique

Insights on Effect of 3N Forces

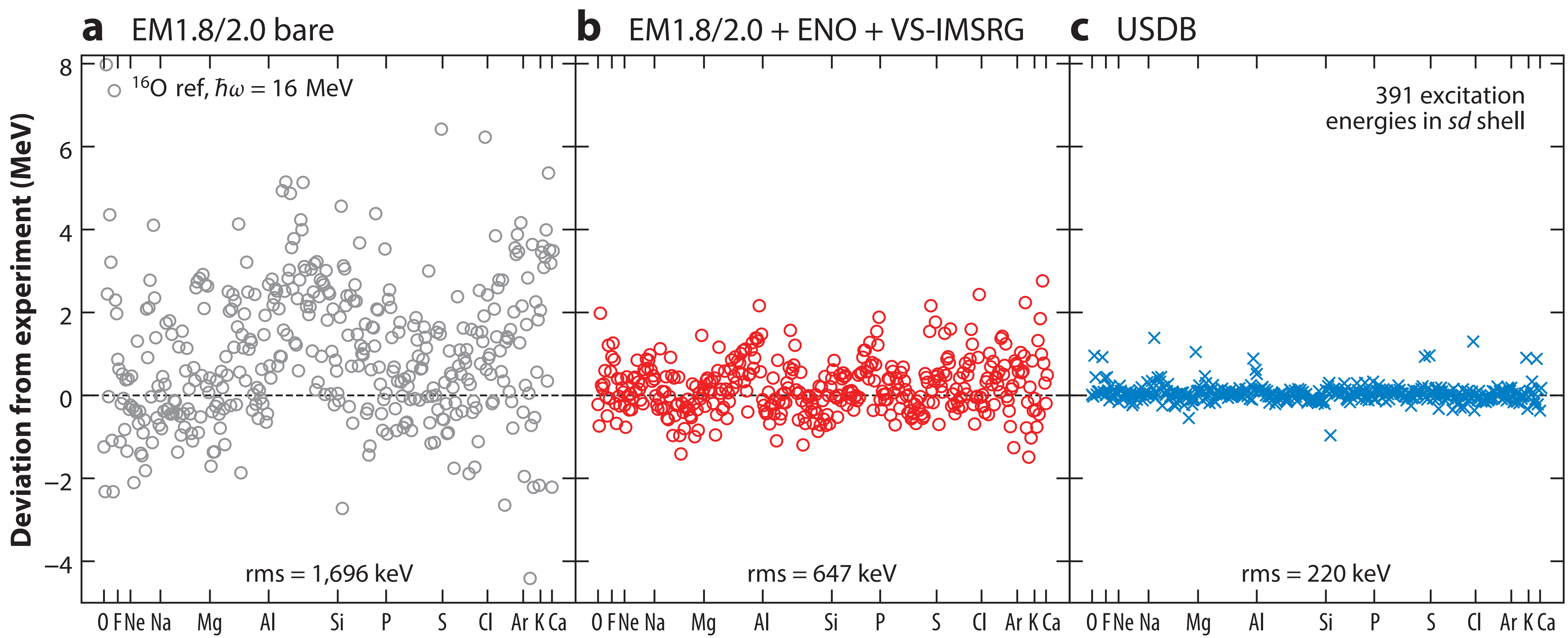
*B. H. Wildenthal, PPNP **11**, 5 (1984); B. A. Brown and B. H. Wildenthal, ARNPS **38**, 29 (1988)*
*B. A. Brown and W. A. Richter, PRC **74**, 034315 (2006)*
*S. R. Stroberg et al., ARNPS **69**, 307 (2019)*



$A^{0.3}$ scaling in USDB / ensemble normal ordering in VS-IMSRG capture **effects of 3N forces amongst valence nucleons**

Description of *sd*-shell States

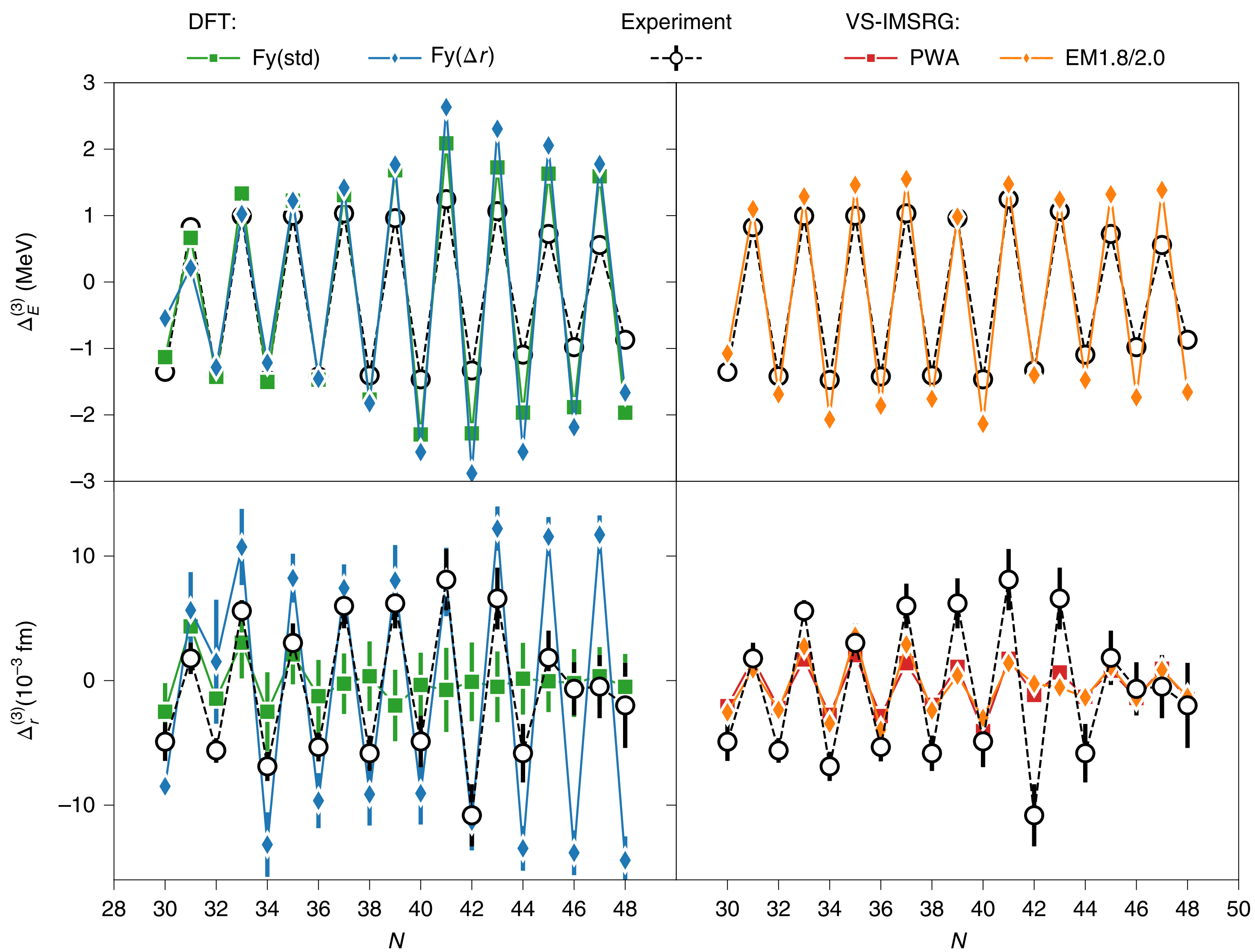
S. R. Stroberg et al., ARNPS **69**, 307 (2019)



Radii

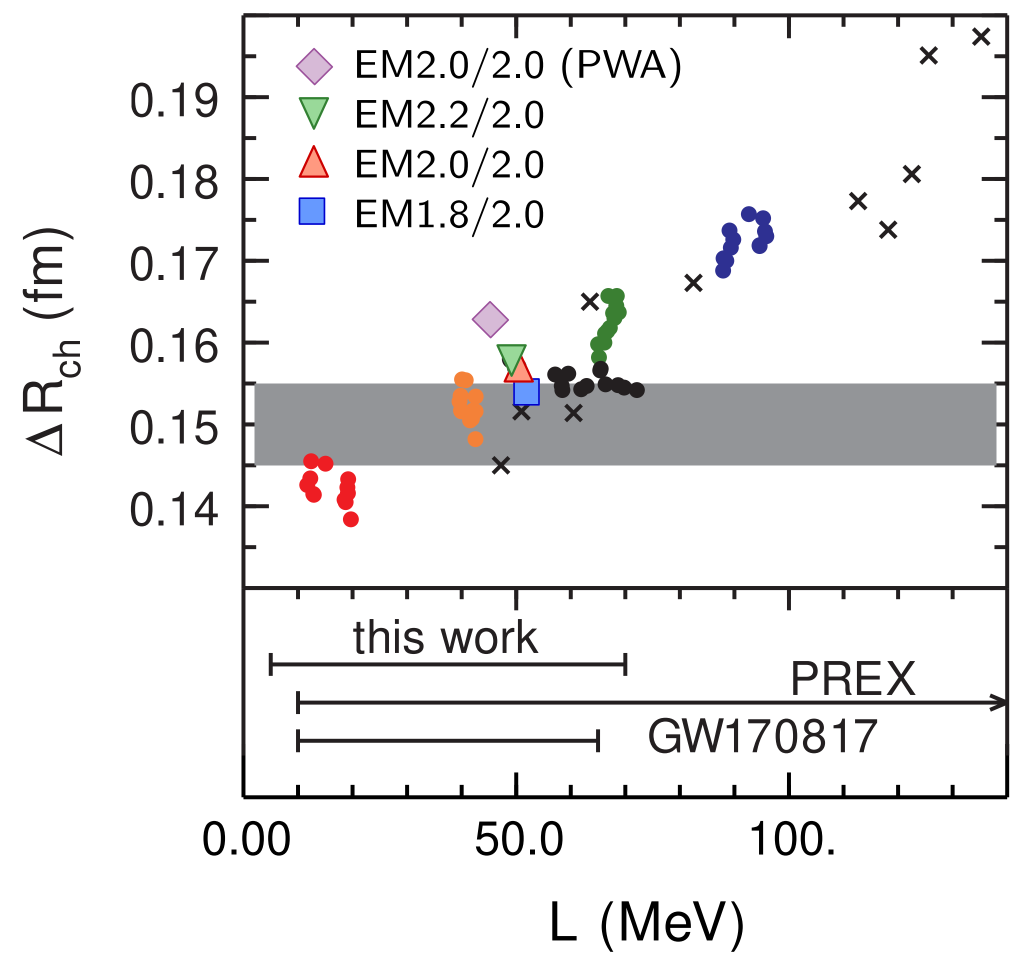
chromium isotopes

*R. de Groote et al., Nat. Phys. **16**, 620 (2020)*



^{36}Ca - ^{36}S

*B. A. Brown et al., PRR **2**, 022305(R) (2020)*

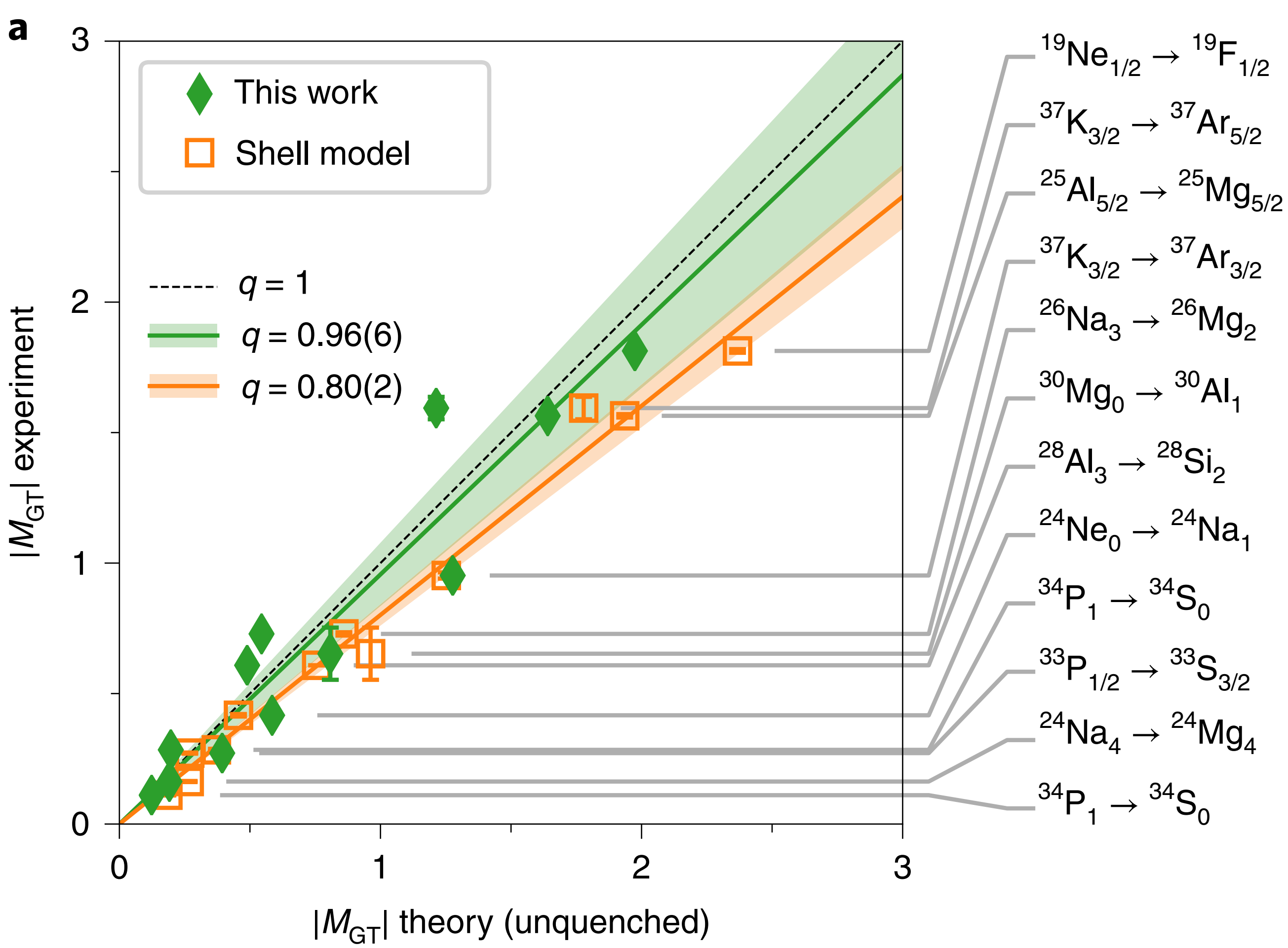


differential observables like the staggering of energies ($\Delta_E^{(3)}$) and radii ($\Delta_r^{(3)}$) or the charge radius difference of mirror nuclei, ΔR_{ch}, are **insensitive** to variations of interaction cutoffs / resolution scale

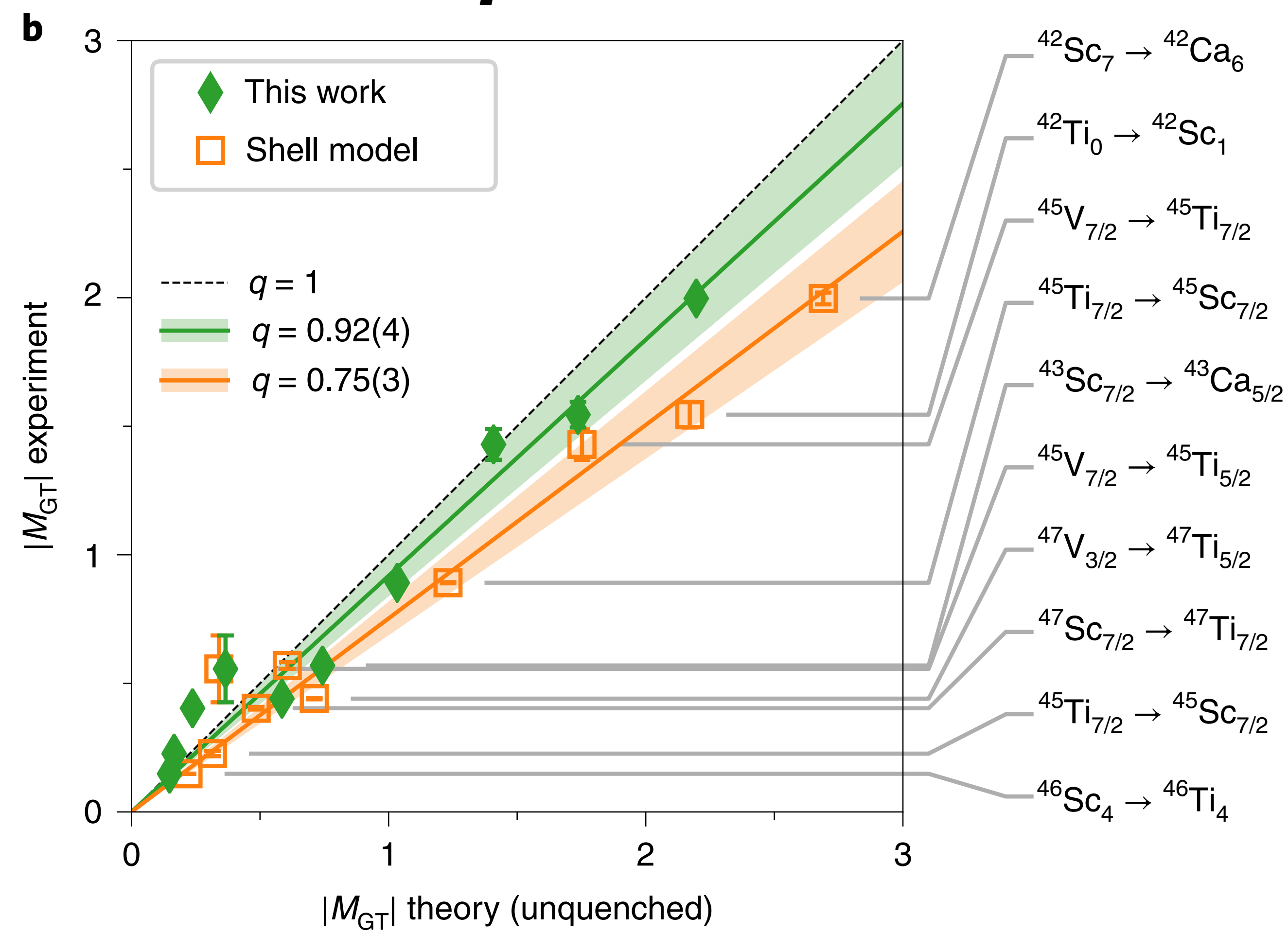
Quenching of Gamow-Teller Decays

P. Gysbers et al., Nature Physics ***15****, 428 (2019)*

sd **shell**



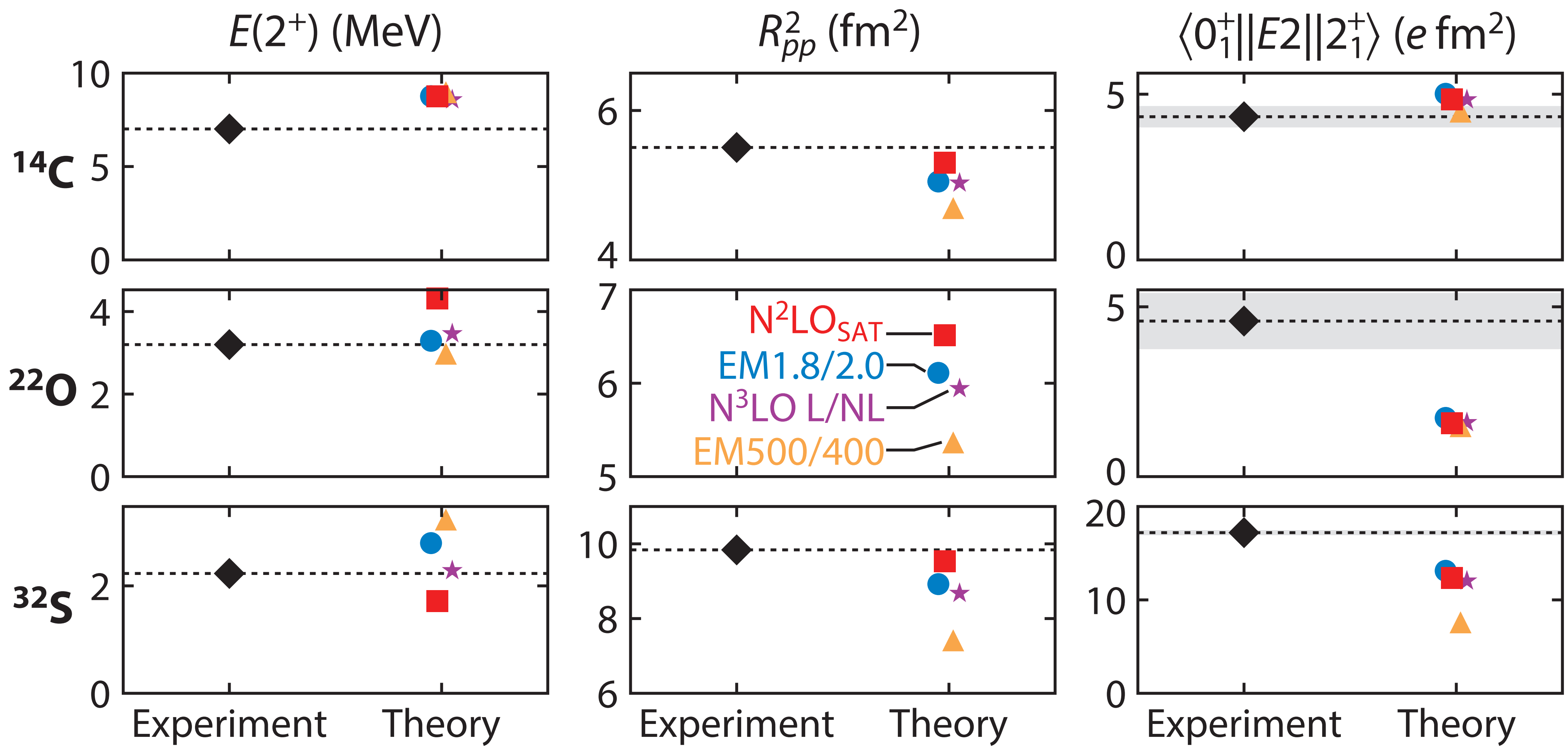
pf **shell**



- **empirical Shell model** calculations require **quenching factors** of the weak axial-vector couling g_A
- **VS-IMSRG** explains this through consistent **renormalization** of transition operator, incl. **two-body currents**

Transitions

*S. R. Stroberg, HH, S. K. Bogner, J. D. Holt, Ann. Rev. Part. Nucl. Sci. **69**, 307 (2019)*
*N. M. Parzuchowski, S. R. Stroberg et al., PRC **96**, 034324 (2017)*
*S. R. Stroberg et al. PRC **105**, 034333 (2022)*



- **B(E2)s too small:** missing collectivity due to intermediate 3p3h, … states that are truncated in IMSRG evolution (**static correlation**)

Capturing Collective Correlations: In-Medium Generator Coordinate Method

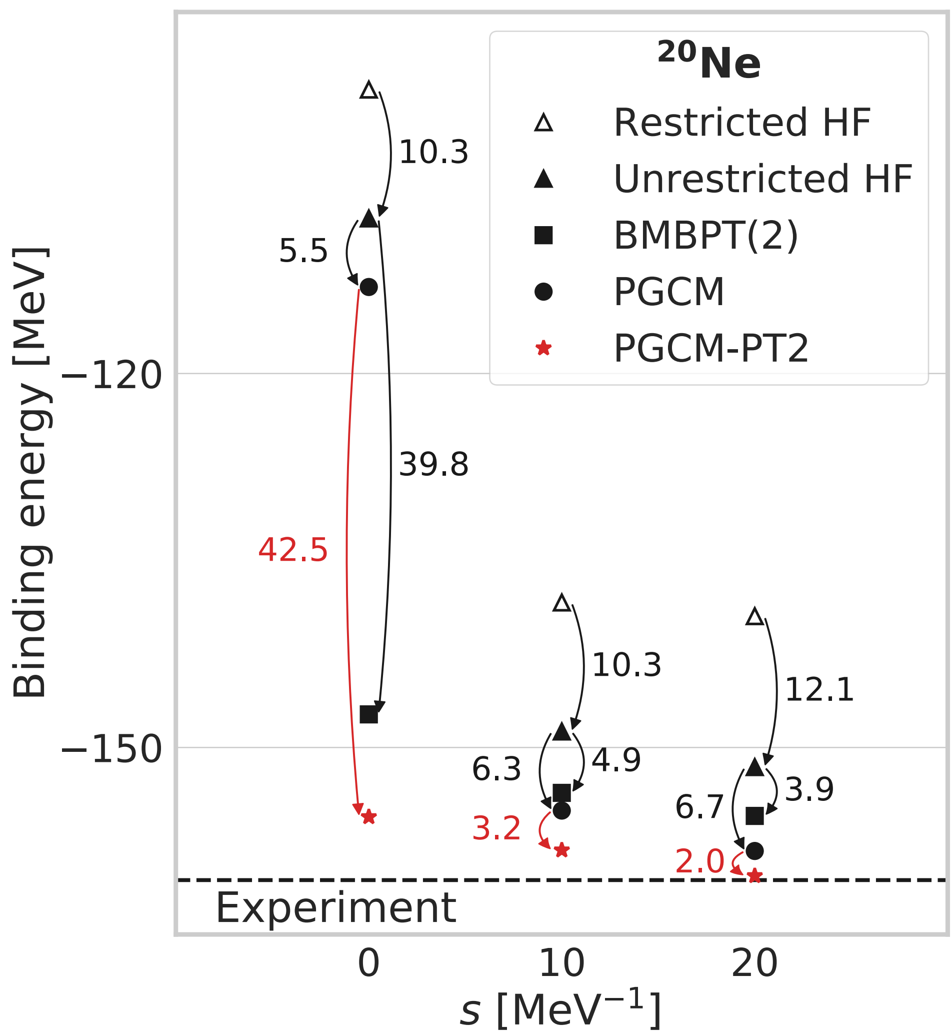
J. M. Yao, A. Belley, R. Wirth, T. Miyagi, C. G. Payne, S. R. Stroberg, HH, J. D. Holt, PRC **103**, 014315 (2021)

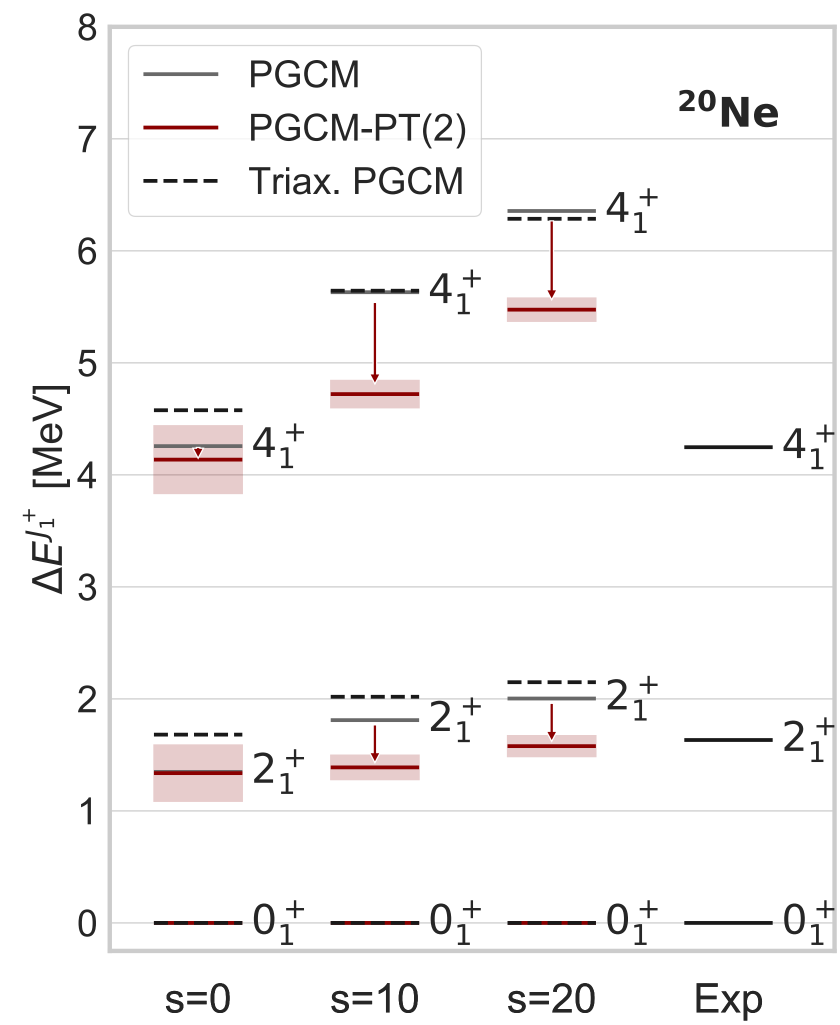
J. M. Yao, B. Bally, J. Engel, R. Wirth, T. R. Rodriguez, HH, PRL **124**, 232501 (2020)

J. M. Yao, J. Engel, L. J. Wang, C. F. Jiao, HH, PRC **98**, 054311 (2018)

Perturbative Enhancement of IM-GCM

M. Frosini et al., EPJA **58**, 64 (2022)



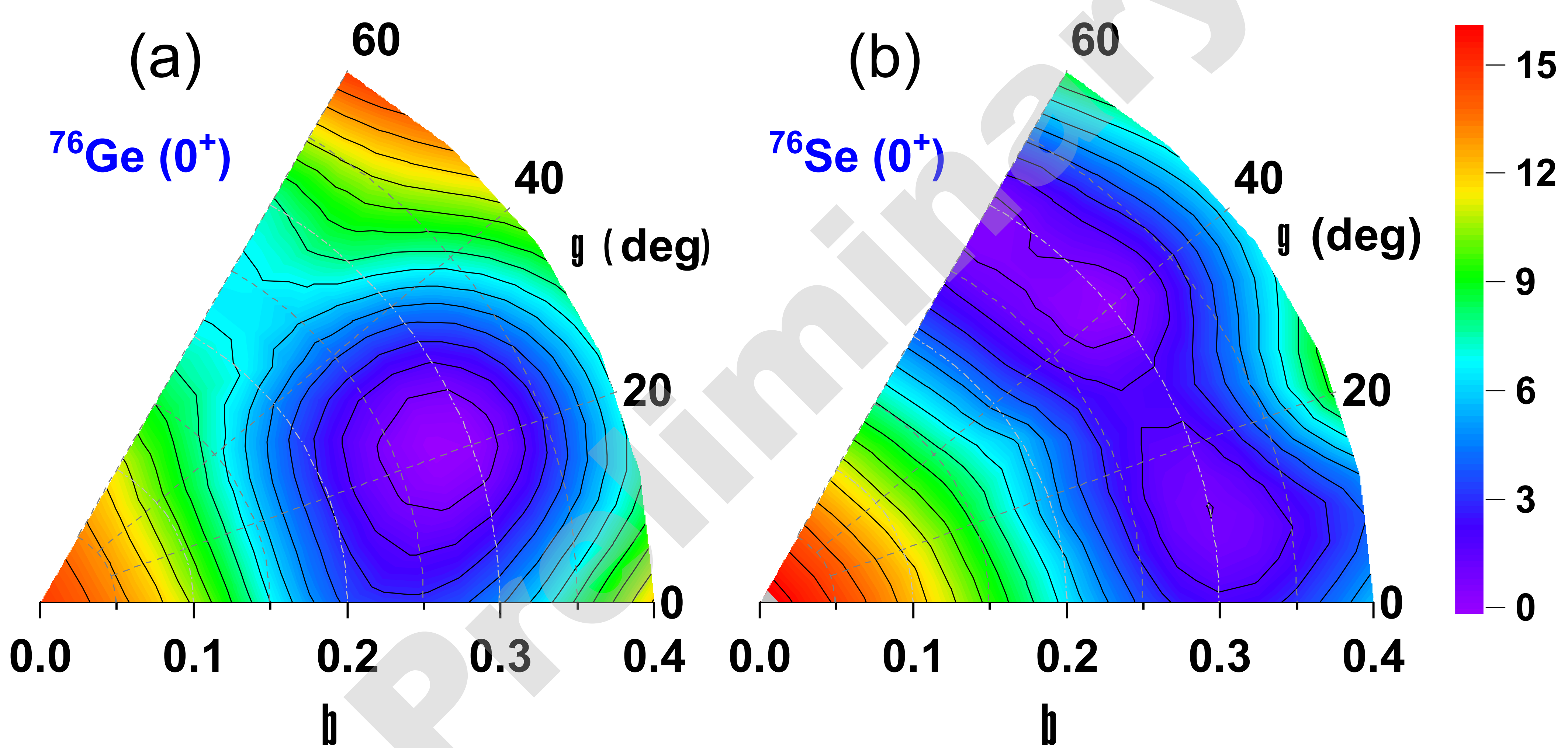


- s-dependence is a **built-in diagnostic tool** for IM-GCM **(not available in phenomenological GCM)**
  - if operator and wave function offer sufficient degrees of freedom, evolution of observables is unitary
- need **richer references and/or IMSRG(3)** for certain observables

^{76}Ge

A. Belley et al., arXiv:2308.15643 (**v2**)

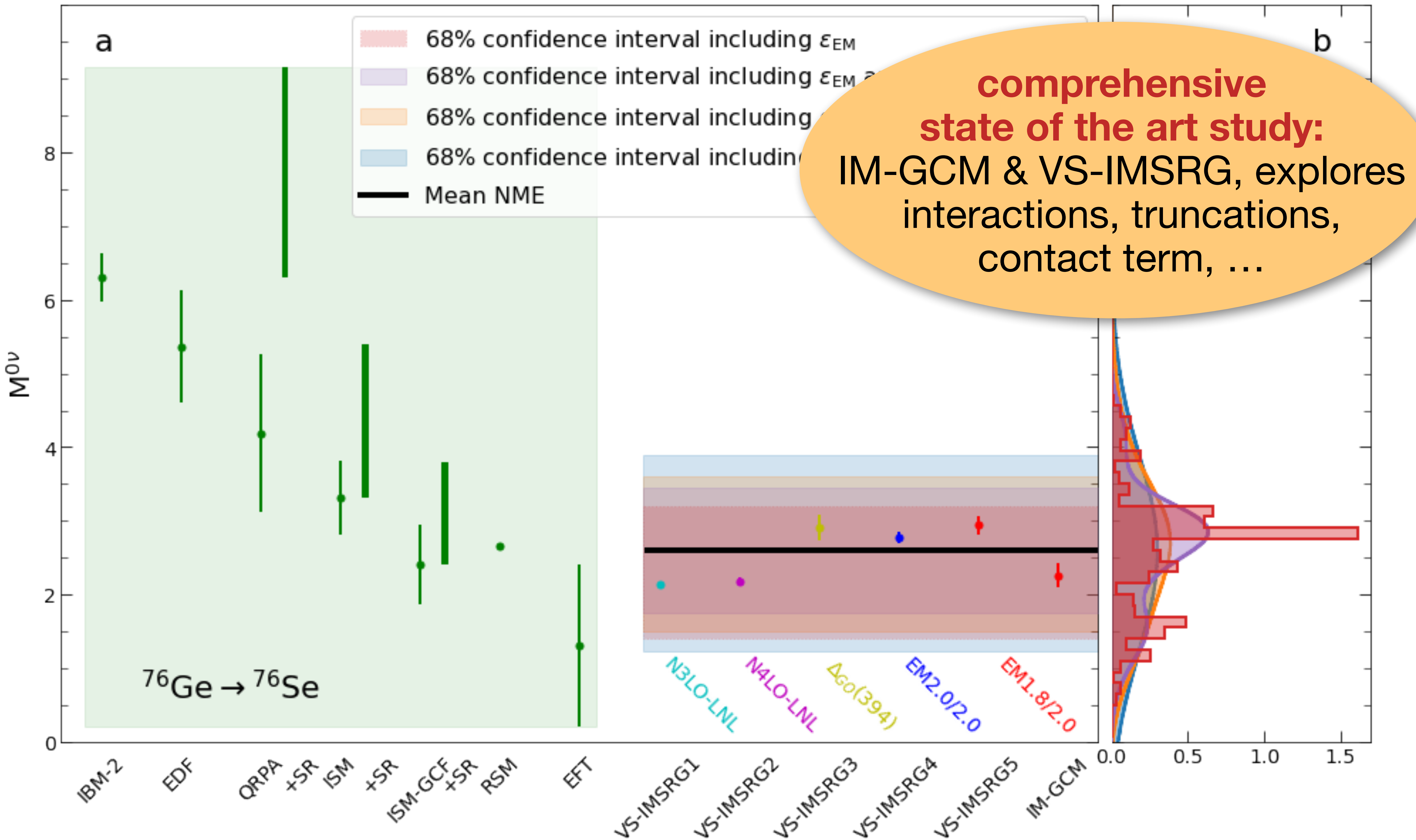
EM1.8/2.0, $e_{\max} = 8$, $E_{3,\max} = 16$, $\hbar\omega = 12\,\mathrm{MeV}$



(also cf. Ayangeaaka et al., PRC 107, 044314)

^{76}Ge

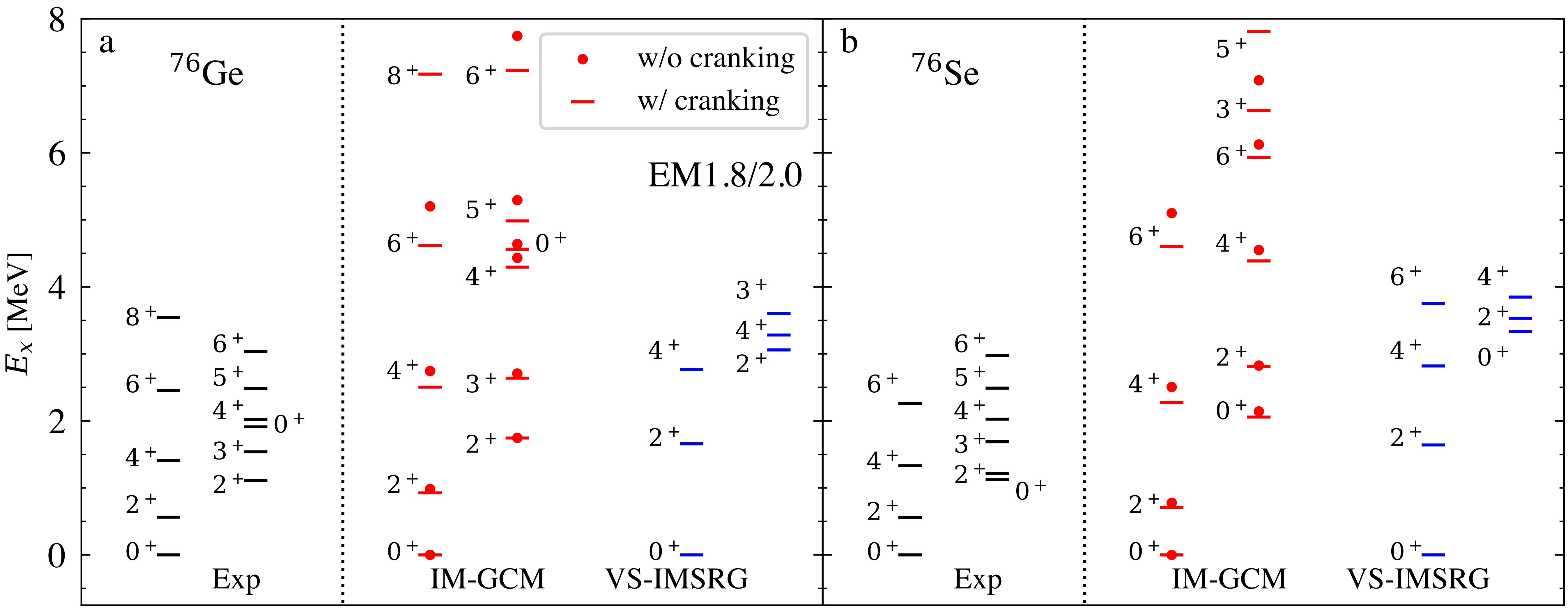
A. Belley et al., arXiv:2308.15643 (**v2**)



comprehensive state of the art study: IM-GCM & VS-IMSRG, explores interactions, truncations, contact term, …

^{76}Ge / ^{76}Se Structure

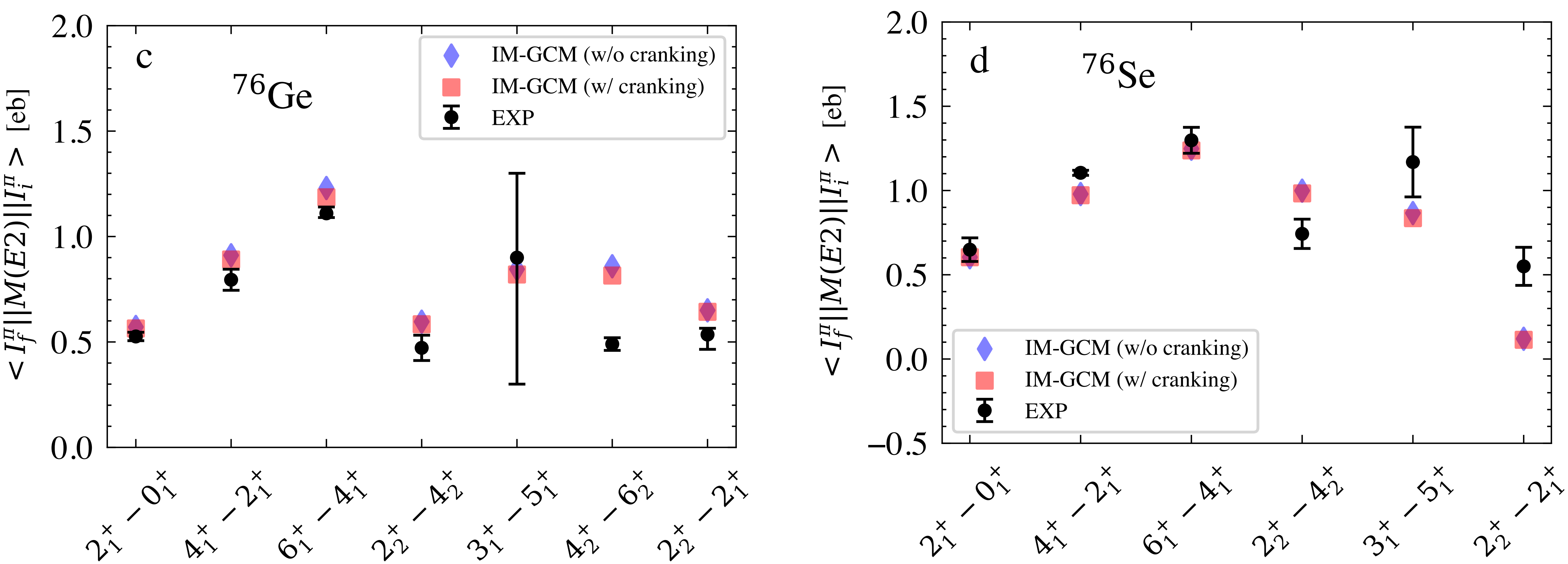
*A. Belley et al., arXiv:2308.15643 (**v2**)*



EM1.8/2.0 NN+3N interaction, $\hbar\omega = 12\,\text{MeV}, e_{max} = 10$

^{76}Ge / ^{76}Se Structure

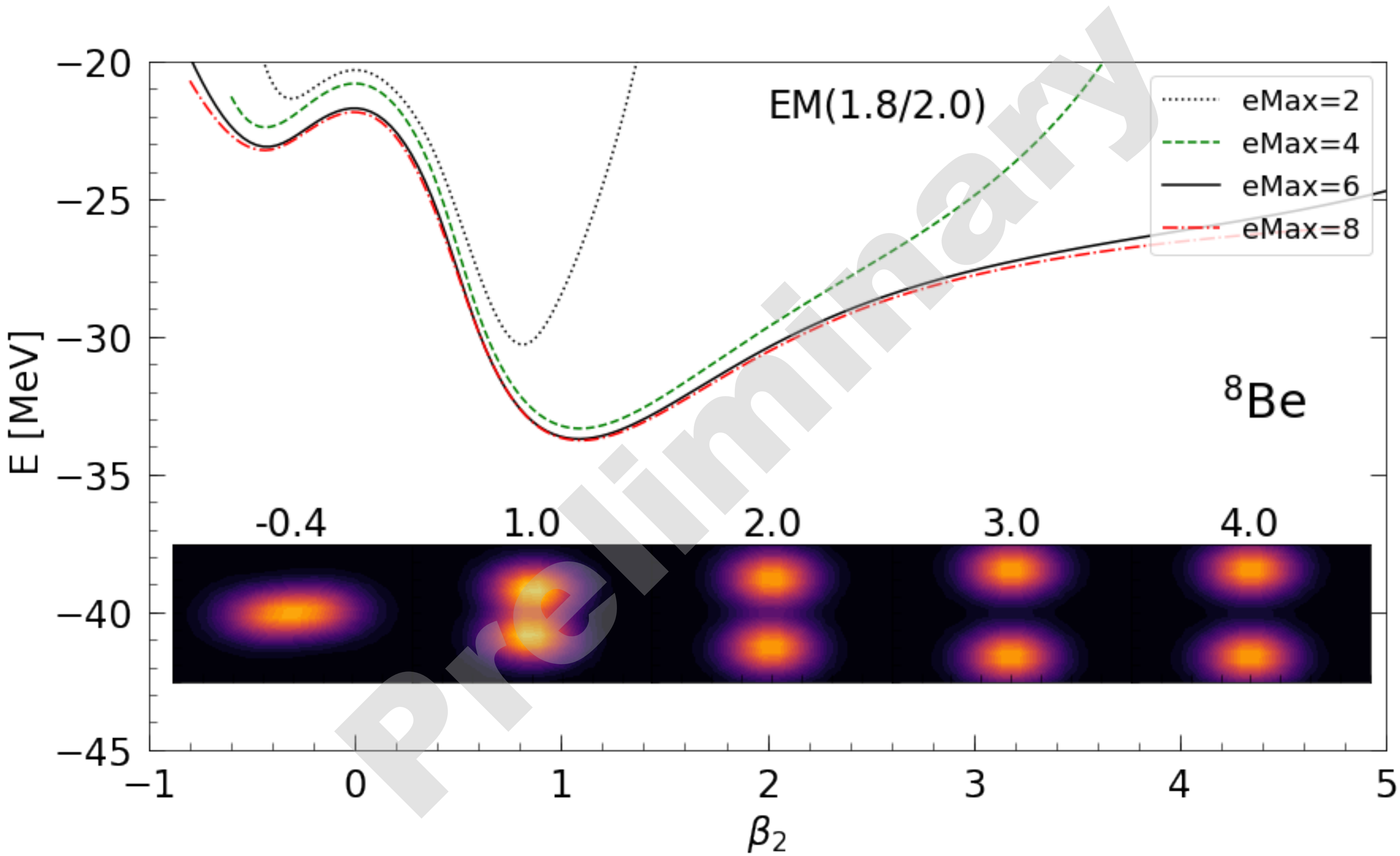
A. Belley et al., arXiv:2308.15643 (**v2**)



EM1.8/2.0 NN+3N interaction, $\hbar\omega = 12\,\mathrm{MeV}, e_{max} = 10$

Cluster Structures: ^{8}Be

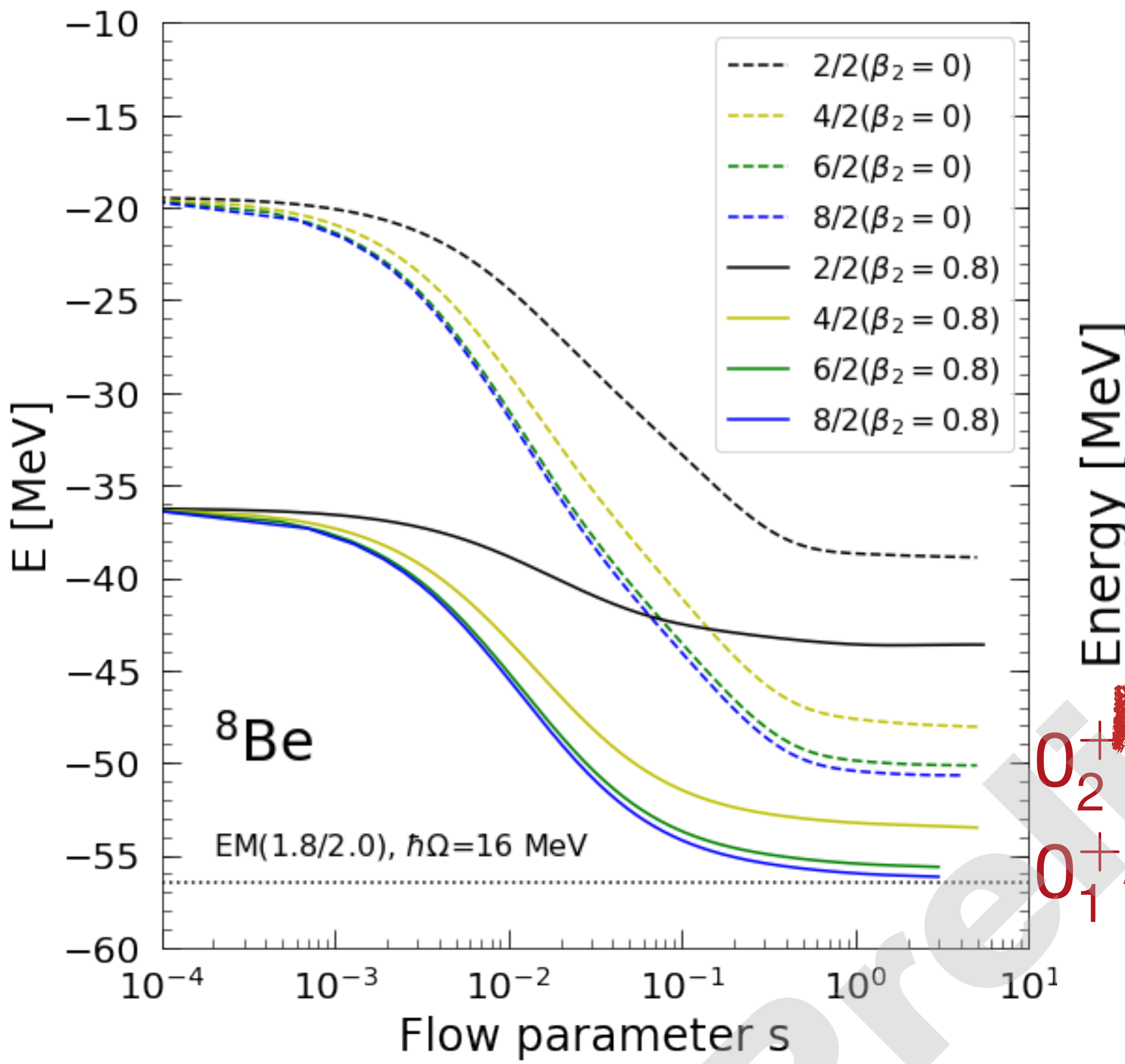
J. M. Yao, R. Wirth, HH, in progress

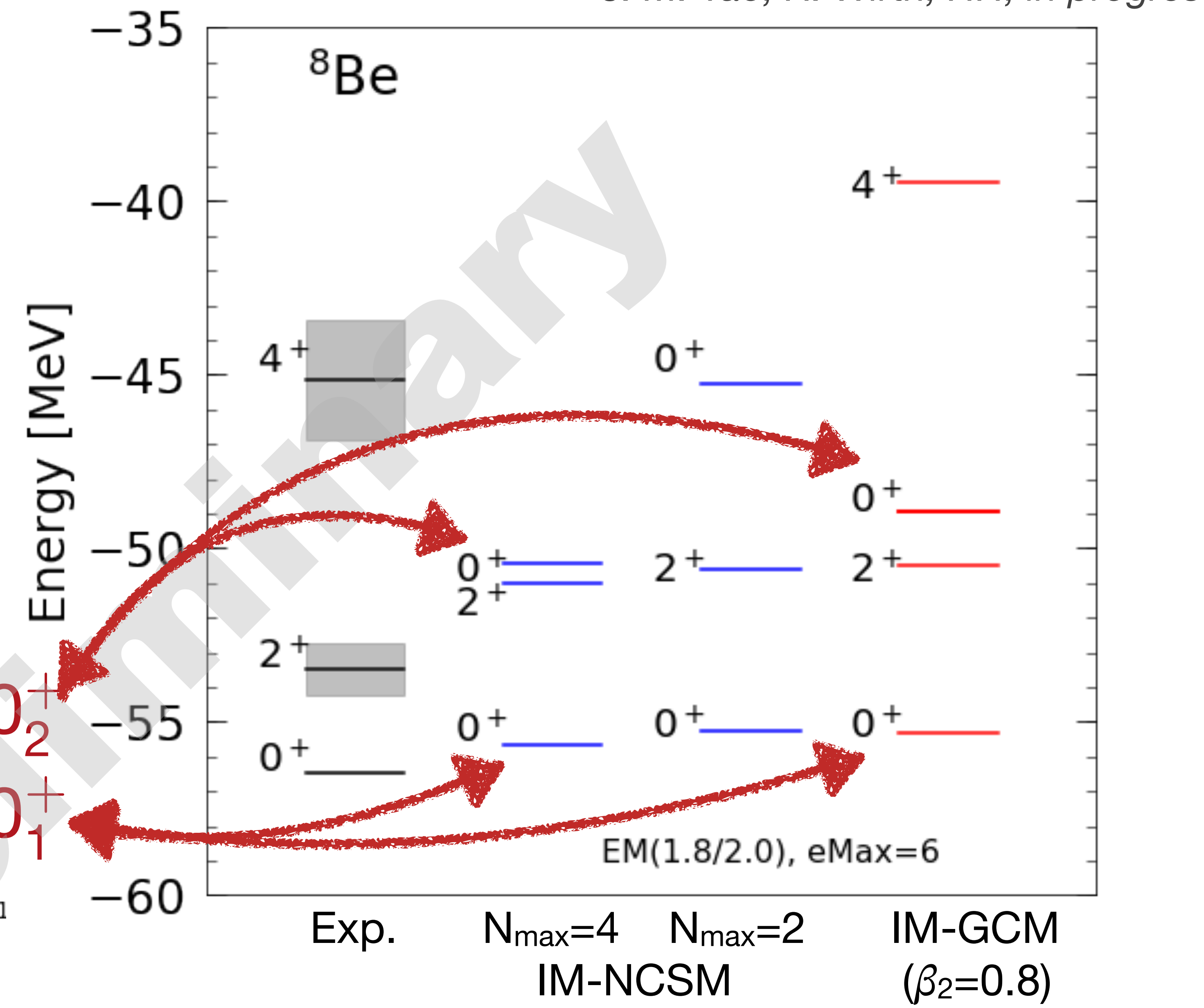


HFB potential energy surface

Cluster Structures: ^{8}Be

J. M. Yao, R. Wirth, HH, in progress





- **Prolate** and **spherical** references flow towards 0_1^+ and 0_2^+ states
  [cf. Sargsyan et al., PRL128, 202503; Caurier et al., PRC64, 051301(R)]
- **seems consistent with IM-NCSM**

Looking Ahead

What Is Next?

- nuclear structure (and reaction) studies with **multiple complementary methods**: IM-GCM, VS-IMSRG, Coupled Cluster, (symmetry-adapted) NCSM(C)…

- **improved truncations:** IMSRG(3) and tailored operator bases

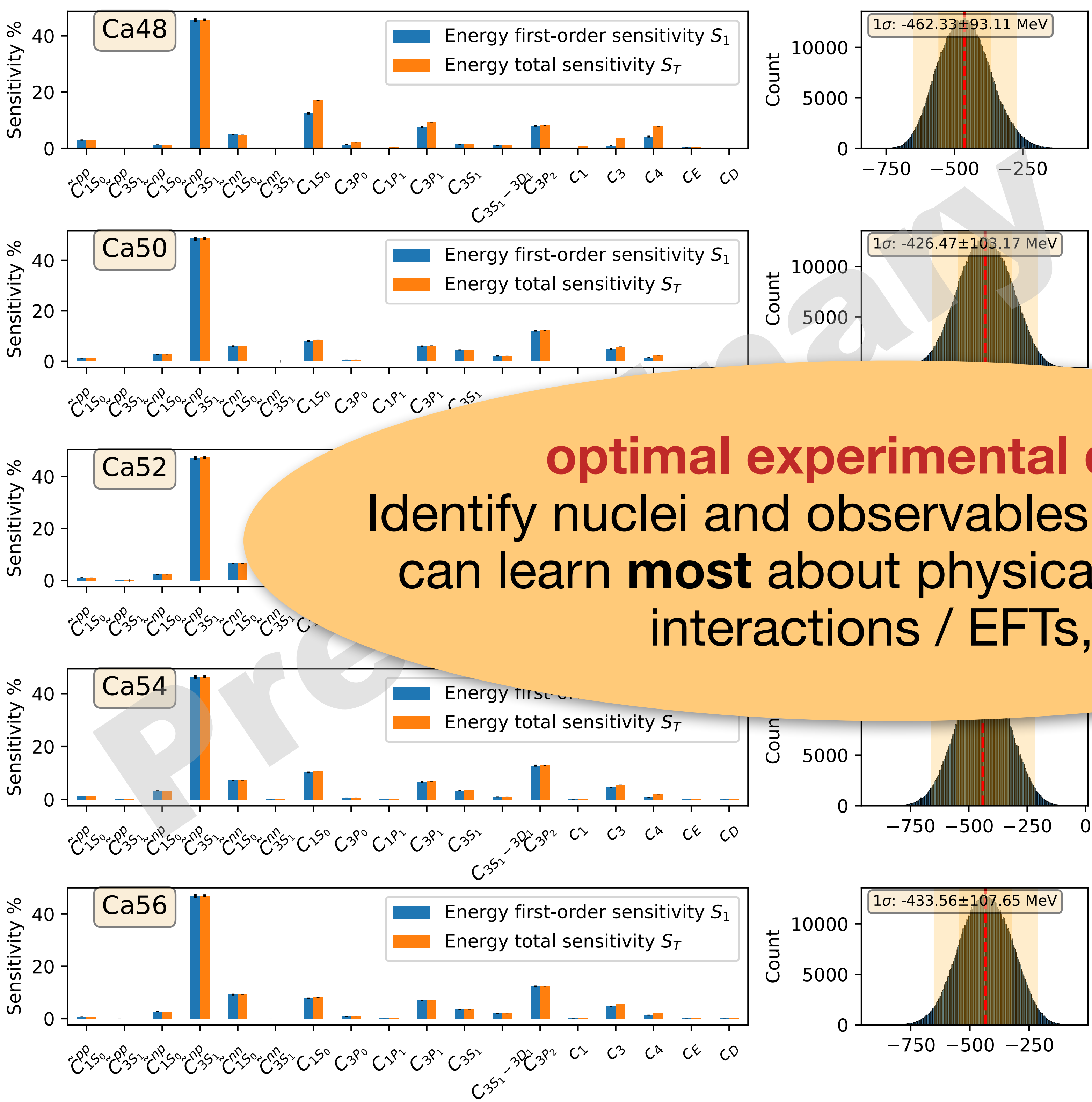
- **accelerate IMSRG & IM-GCM** (GPUs, factorization, Machine Learning, …)
  [A. M. Romero et al., PRC 104, 054317; X. Zhang et al., PRC 107, 024304]

- **Uncertainty Quantification / Sensitivity Analysis**

  - need cheap **surrogate models (emulators)**

Emulation for Operators (IMSRG)

***J. Davison, J. Crawford**, S. Bogner, HH, in preparation*



- non-invasive "physics-driven" emulator
- NNLO$_{sat}$, NN+3N
- = 12,
  4
  samples
- **5+ order of magnitude reduction in computational effort**

optimal experimental design:
Identify nuclei and observables from which we can learn **most** about physical phenomena, interactions / EFTs, …

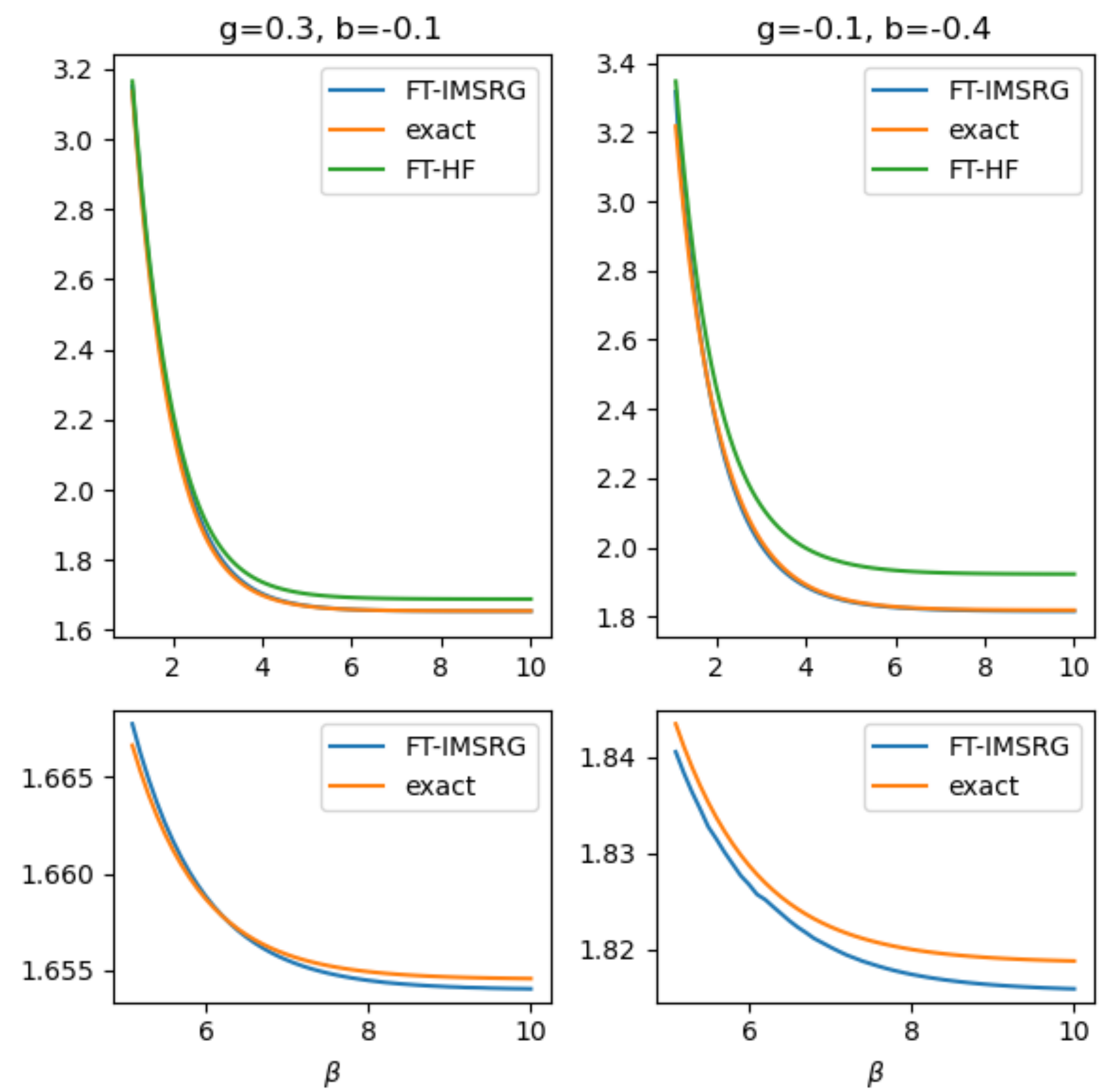
Preview: Finite-Temperature IMSRG

- formalism and benchmark paper **out soon**
- implementation for **realistic nuclei and chiral interactions** complete, under validation
- expect first **applications to structure, beta decays** within next 1-2 years

The In-Medium Similarity Renormalization Group at Finite Temperature

Isaac G. Smith, Heiko Hergert, Scott K. Bogner
Facility for Rare Isotope Beams, Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824

The study of nuclei at finite-temperature is of immense interest in nuclear astrophysics. Many *ab initio* methods for determining properties of nuclei at zero-temperature have been developed over the past few decades. We expand one such method, the In-Medium Similarity Renormalization Group (IMSRG), to finite temperature. The implementation of the finite-temperature IMSRG (FT-IMSRG), including the implementation of finite-temperature Hartree-Fock, is detailed. Using an exactly-solvable toy model, we show that the FT-IMSRG can accurately determine the energetics of nuclei at finite temperature. The effect of model parameters on the FT-IMSRG's accuracy is



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UT Knoxville & Oak Ridge National Laboratory

R. J. Furnstahl
The Ohio State University

and everyone I forgot to list…

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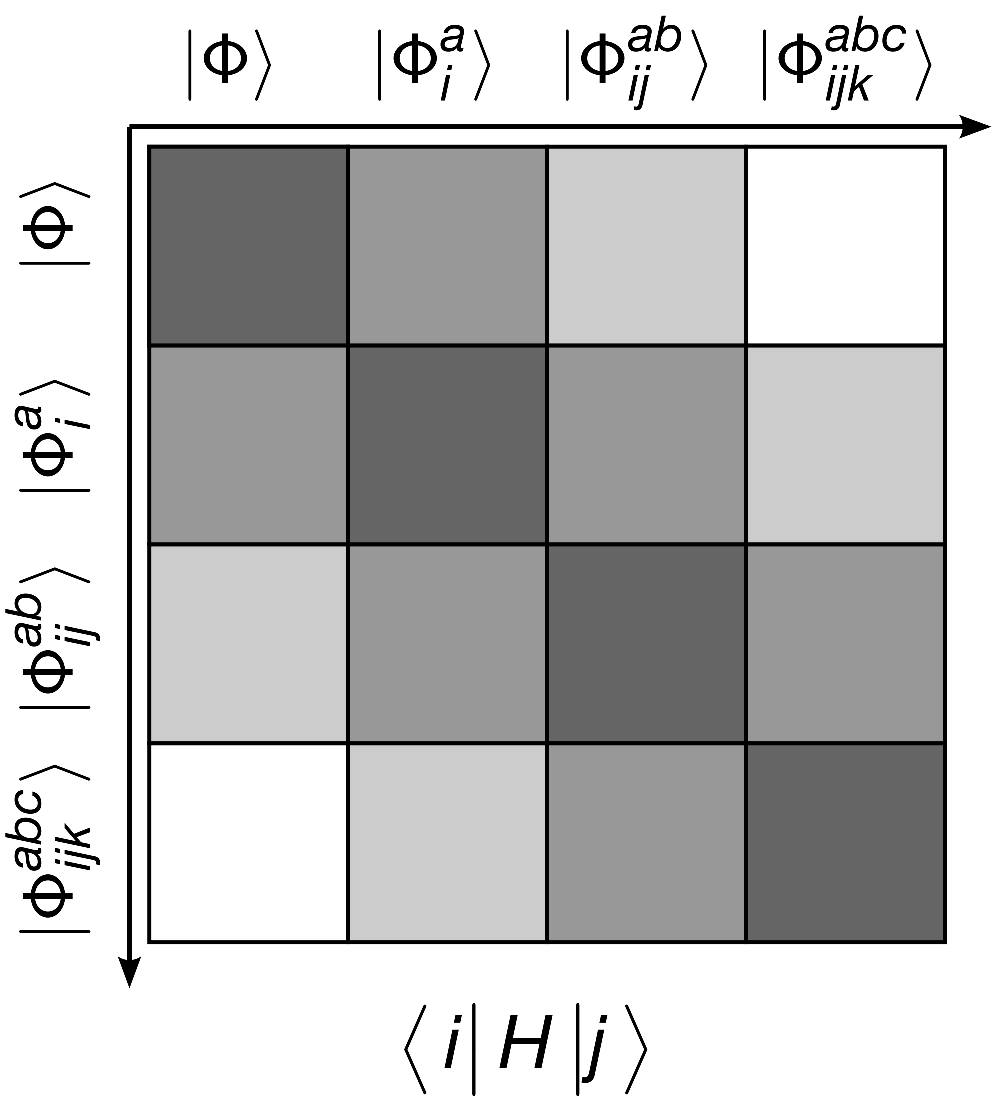
Supplements

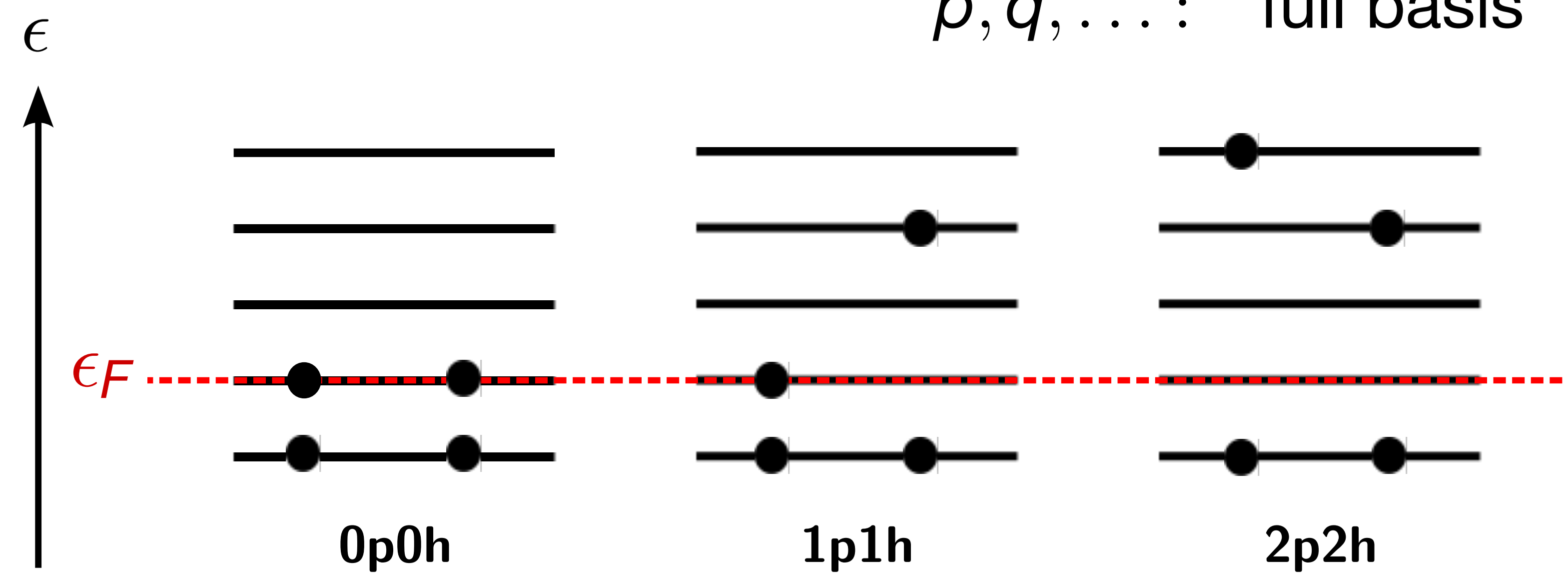
Transforming the Hamiltonian



$a, b, \ldots : \quad \epsilon > \epsilon_F$

$i, j, \ldots : \quad \epsilon \leq \epsilon_F$

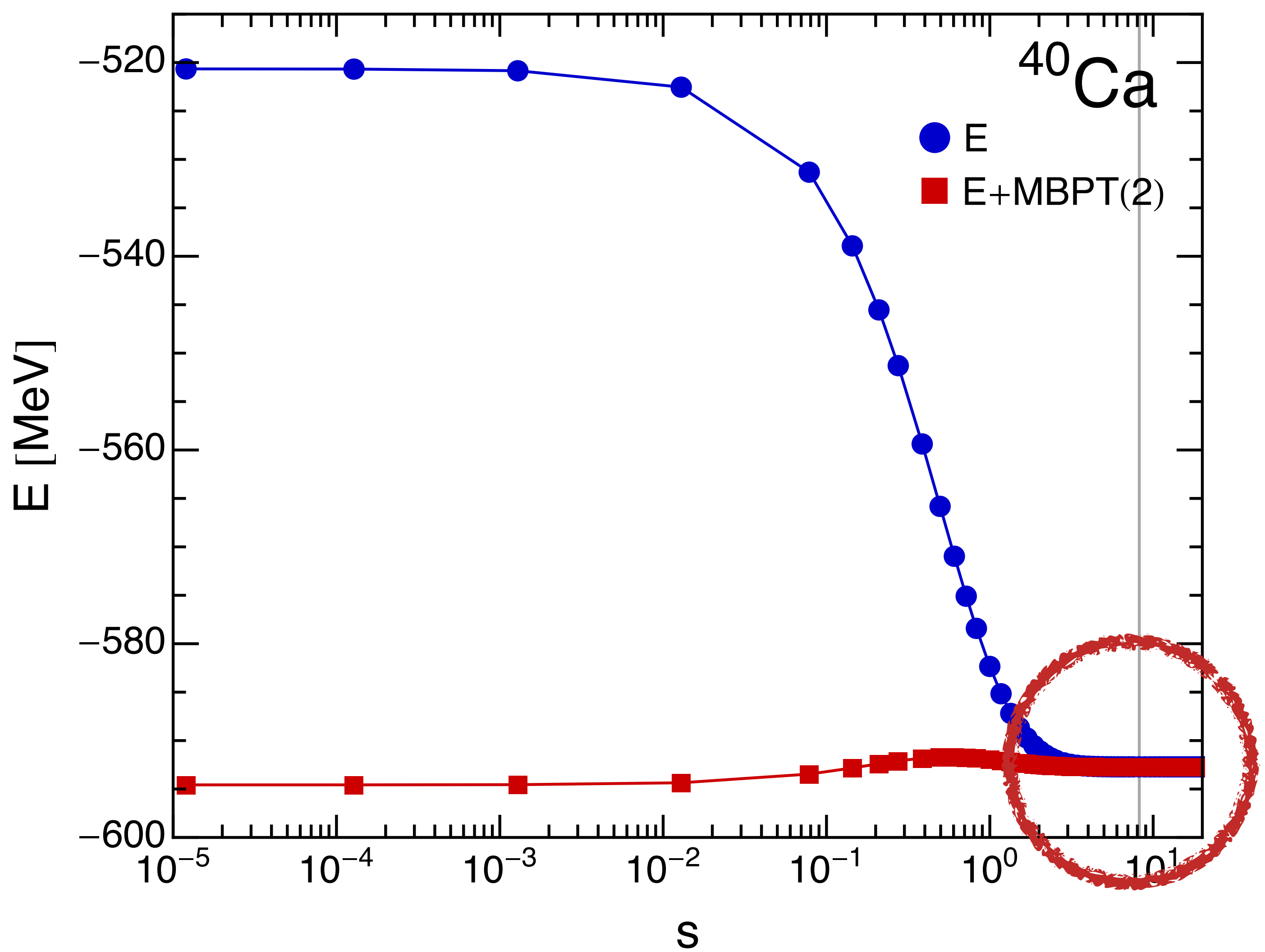
$p, q, \ldots :$ full basis

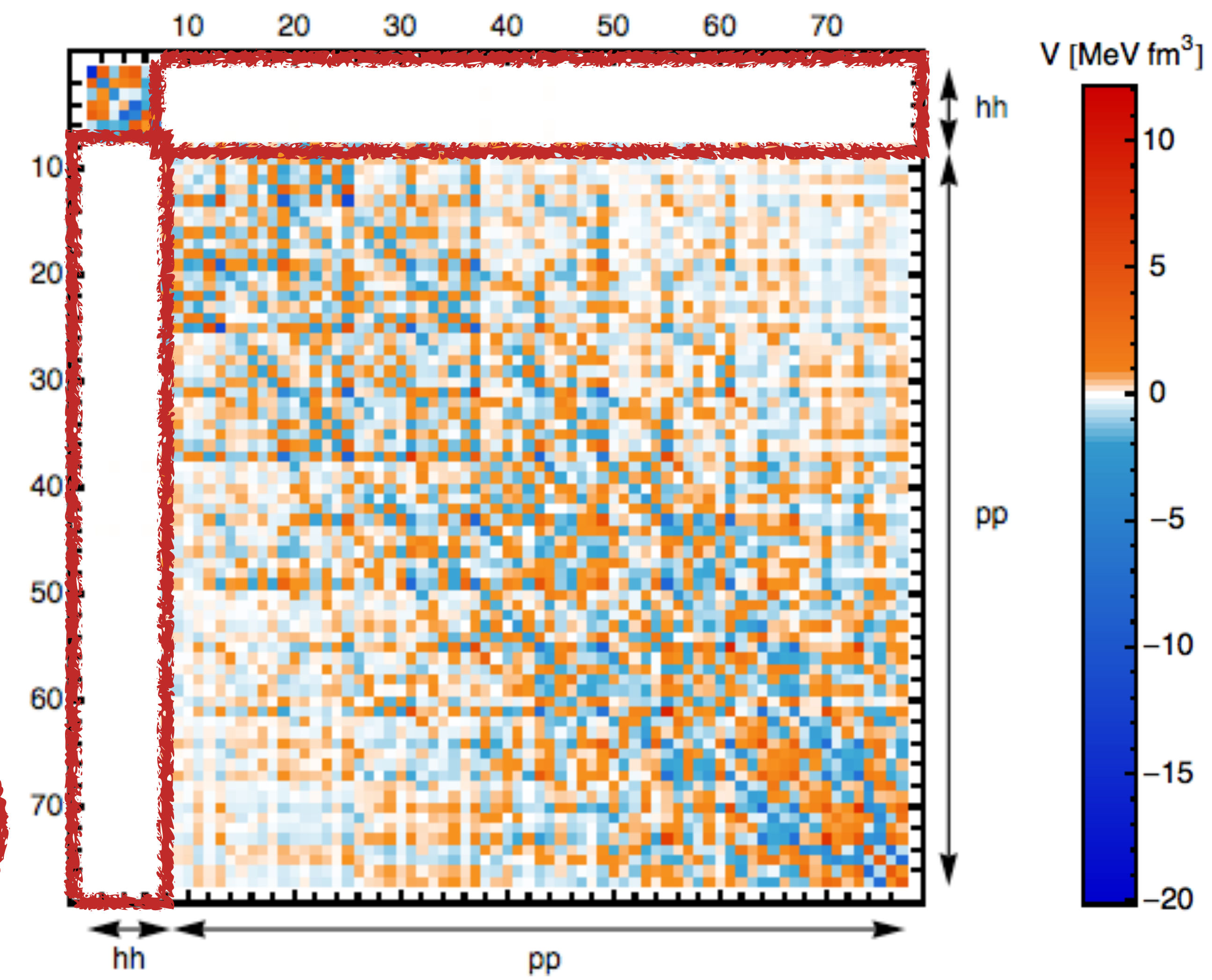


excitations relative to reference state: **normal-ordering**

- reference state: **single Slater determinant**

Decoupling



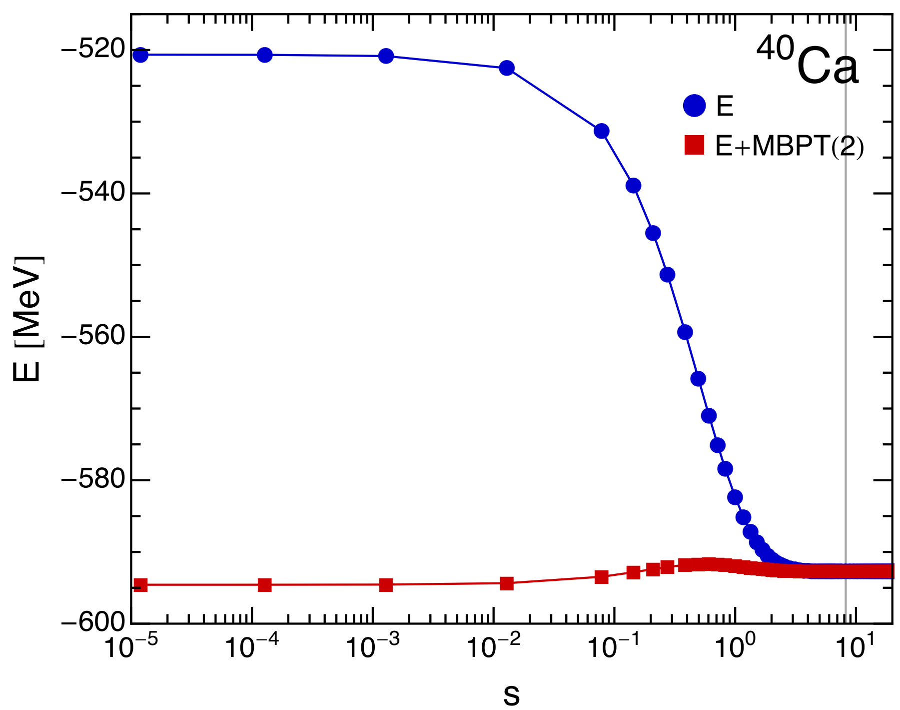


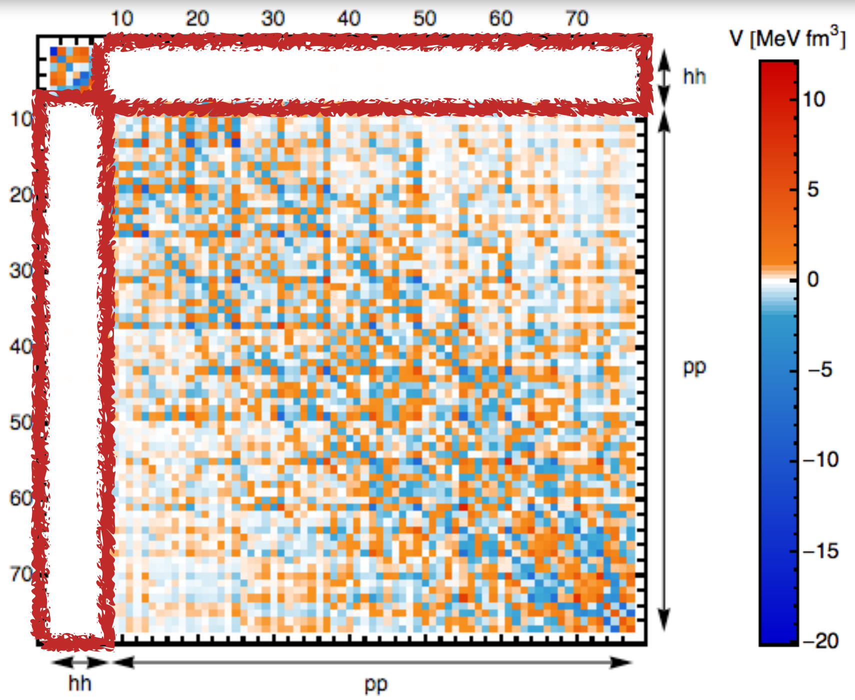
N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

non-perturbative resummation of MBPT series **(correlations)**

off-diagonal couplings are rapidly driven to zero

Decoupling





N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

- absorb correlations into **RG-improved Hamiltonian**

$$U(s)HU^{\dagger}(s)U(s)\left|\Psi_n\right\rangle = E_n U(s)\left|\Psi_n\right\rangle$$

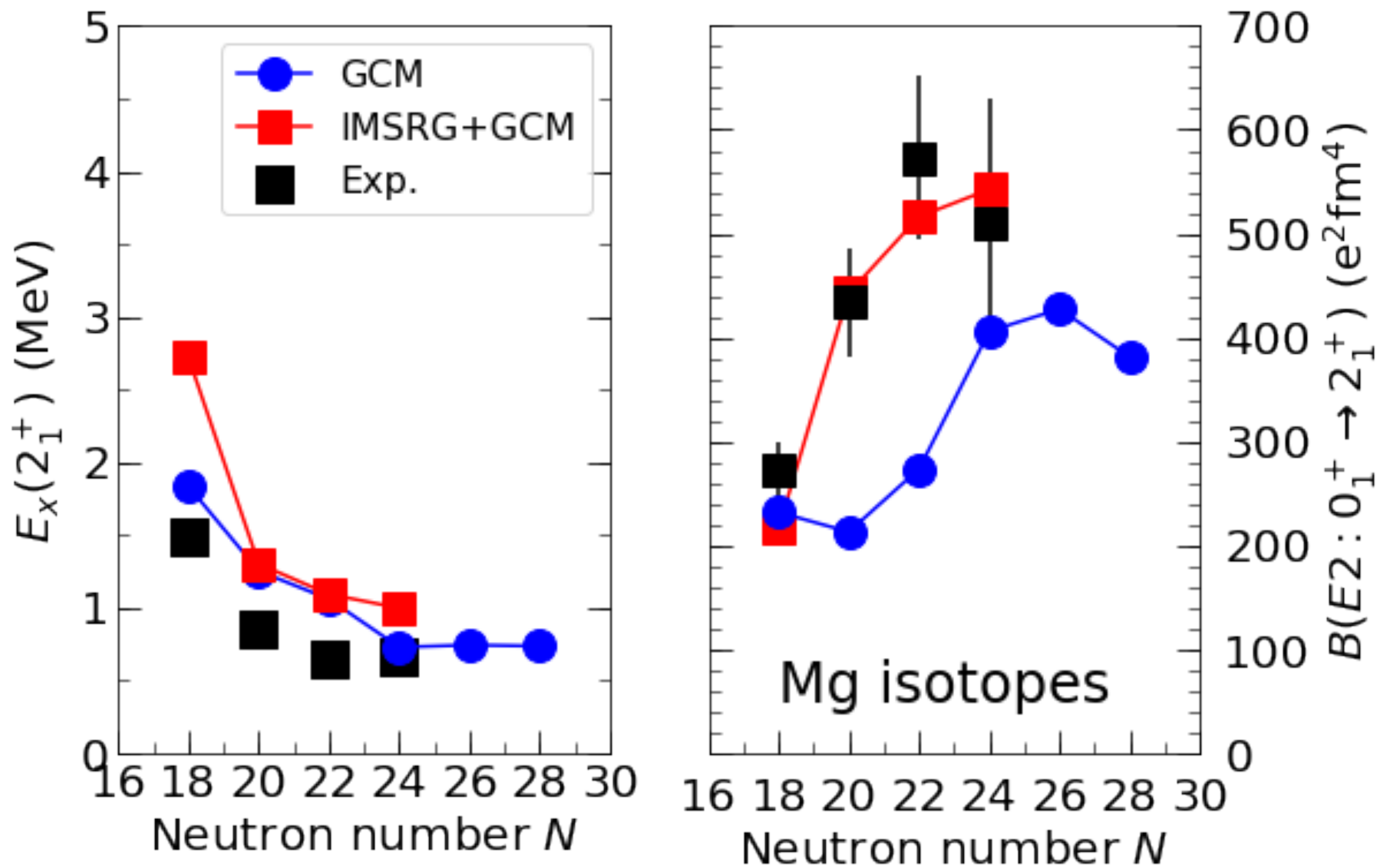
- reference state is ansatz for transformed, **less correlated** eigenstate:

$$U(s)\left|\Psi_n\right\rangle \stackrel{!}{=} \left|\Phi\right\rangle$$

Magnesium Isotopes

J. M. Yao, HH, in preparation

EM1.8/2.0

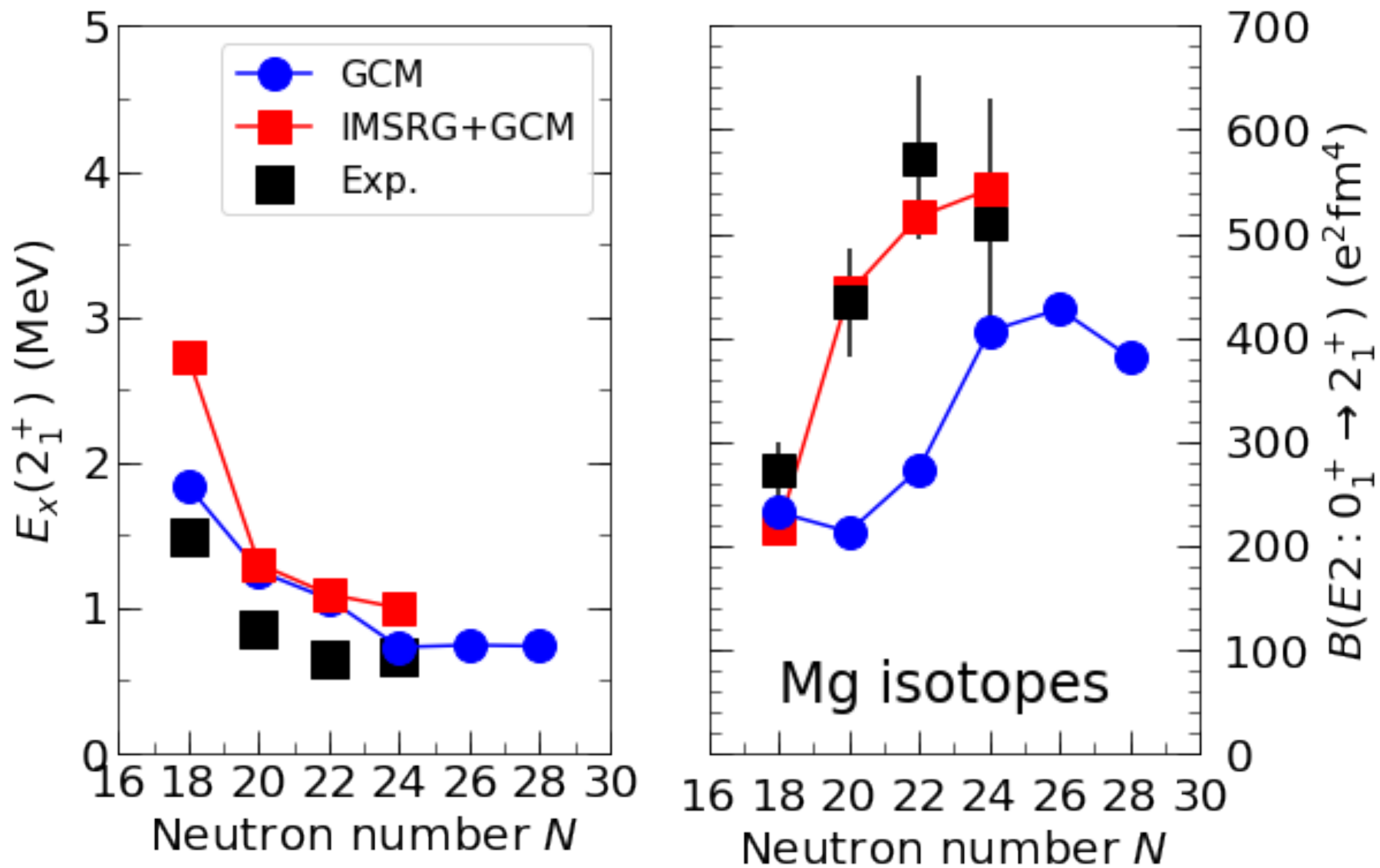


- much **improved B(E2)** values compared to standard GCM or VS-IMSRG calculations: IM-GCM captures **dynamical and static correlations**!

Magnesium Isotopes

J. M. Yao, HH, in preparation

EM1.8/2.0



$$O = O^{(1)} \xrightarrow[s\to\infty]{} O(s) = O^{(1)}(s) + \underbrace{O^{(2)}(s) + \ldots}_{\text{induced contributions}}$$

- **induced 2B quadrupole operator is small (~5%),** contrary to typical VS-IMSRG (~50%): GCM reference equips operator basis with better capability to capture collectivity